Abstract—During the course of expansion of steam in turbines, the vapour first supercools and then nucleates to become a two phase mixture. Formation of the liquid phase causes thermodynamic and aerodynamic losses in steam turbines. Therefore the study of two phase flow is undeniably an important issue. Despite a huge research effort, many uncertainties remain and it is concluded that the predictive accuracy required for engineering calculation is not yet achievable with a theory derived from first principles. The areas that require most attention relate to the properties of small molecular cluster such as surface tension at small droplet sizes, the value of the condensation coefficient and the equation of state for supercooled steam to calculate isentropic exponent whose exact amount is still an issue open to debate. In this article by applying Levenberg-Marquardt’s reverse modeling method for capturing experimental data of shock and it specifies the optimum amount for these three parameters has been achieved that makes possible a better and more precise analysis of two phase flow for predicting condensation in steam nozzles.

Keywords—reverse, Levenberg-Marquardt, surface tension, condensation coefficient, two phase.

I. INTRODUCTION

Progress in the development of the steam turbines brings about a renewal of interest in wetness associated problems. The fluid temperature in LP turbines decreases due to the steam expansion. Therefore, the superheat vapour crosses the saturation line and enters the two phase region. Due to the high velocity of the steam flow, it is still single-phase that is called supercooled vapour. This situation continues to the Wilson point, where the supercooled steam cannot continue and the fluid starts nucleating and liquid droplets with small diameters are formed. This growing droplets release their latent heat to the flow and this heat addition to the supersonic flow cause a pressure rise called condensation shock. Because of irreversible heat transfer in this region the entropy increase tremendously and cause thermodynamic and aerodynamic losses.[1]-[2]. The nucleation model presented in this research is a homogenous nucleation. In this kind of nucleation, condensation occurs without any impurity[3]-[8].

There is a variety of techniques in solving reverse engineering problems that some of them have been mentioned in the following:

i. Levenberg-Marquardt’s method; for estimating unknown parameter

ii. Conjugate Gradient method; for estimating unknown parameter

iii. Conjugate Gradient with Adjoint; for estimating unknown sequence

In this paper we wish to observe the fluid from the flowing points of view for optimizing the process and want to use Levenberg-Marquardt’s method and in order to investigate condensing steam flow a two-phase Eulerian-Lagrangian model is used where conservation equation for the two phase mixture are solved in a Eulerian frame of origin, but nucleation and droplet grows are calculated following fluid particles in steady one dimensional flows. The flow is considered as a whole, the change in momentum of the system across centerline can be written. Considering the flow of energy into and out of the control volume the energy equation can be also written. It represents the heat released to or absorbed from the flow by condensation onto or evaporating from the droplets. Two phase effects enter into these equations through the density and enthalpy. These are non-equilibrium mixture quantities and therefore depend on the mass fraction of the liquid and on the vapour subcooling. Equations of momentum and energy are combined with equations of state and Mach number. Hence four unknowns temperature, pressure velocity and density can be reached[4]-[12].

II. MAIN FLOW EQUATIONS

By considering the steady one-dimensional flow over an incremental distance $dx$ along the channel, the fundamental equation of flow can be written as:

$$\frac{d\rho}{\rho} = \frac{A}{\rho} \left( \frac{du}{u} - \frac{dW}{W} \right) = 0$$

(1)

where $W$ is the overall mass flow rate.

State Equation:

$$\frac{P}{\rho RT} = 1 + B_1 \rho \mu + B_2 \rho \mu^2 + B_3 \rho \mu^3 + B_4 \rho \mu^4 + B_5 \rho \mu^5$$

(2)

where $B$ parameters are viral coefficients; these are functions of temperature as given in Appendix A [5].
\[ \frac{dP}{T} - X \frac{dP}{\rho_c} - \frac{dT}{T_c} = 0 \]

where
\[
X = \frac{\rho_c}{P} \left( \frac{\partial P}{\partial \rho_c} \right)_{T_c} = 1 + 2B \rho_c^2 + 3B \rho_c^2 + 4B \rho_c^2 + 5B \rho_c^2 + 6B \rho_c^2
\]

\[
Y = \frac{T_c}{P} \left( \frac{\partial P}{\partial T_c} \right)_{\rho_c} = 1 + B \rho_c^2 + B \rho_c^2 + B \rho_c^2 + B \rho_c^2 + B \rho_c^2
\]

\[
\frac{1}{\rho_c} \frac{d\rho_c}{dt} = \frac{1}{L} \frac{dL}{dW} + \frac{1}{\rho_c} \frac{d\rho_c}{dt} + \frac{1}{L} \frac{dL}{dW}
\]

\[ Z = Ma^2 = \frac{u^2}{\sqrt{\rho_c}} \]

Differentiating the equation (5) leads to:
\[
\frac{dZ}{Z} = \frac{2Ma^2}{u} \frac{du}{\rho_c} \frac{d\rho_c}{dt} \frac{dp}{p}
\]

Momentum Equation

Considering the flow as a whole, the change in momentum of the system across \( dx \) can be written as:
\[ AdP + A \frac{f \rho_c u_c^2}{2D_y} dx = -d[W_L u_L + W_I u_I] \]

Expanding this equation, denoting \( dW_0 = -dW_L \) and dividing by \( A \times P \), regarding \( (u_c - u_L) \) \( dW_L \) small in comparison with others and re-arranging:
\[
\frac{dP}{P} = \frac{f \rho_c u_c^2}{2P} \frac{dW_0}{D_y} A \frac{u_c}{u_c} \frac{dW_L}{Ap} \frac{u_c}{u_c} \frac{dW_L}{Ap} \frac{u_c}{u_c}
\]

Energy Equation

Considering the flow of energy into and out of the control volume and assuming the heat loss through the sides of the duct to be small, the energy equation can be written as:
\[ d \left[ (W - W_L) h_L + \frac{u^2}{2} \right] + W_L (h_c + \frac{u^2}{2}) = 0 \]

Since the phase change occurs within the control volume, the term \( dW_L (h_c - h_L) \) will appear while expanding this equation. It represents the heat released to or absorbed from the flow by condensation onto or evaporating from the droplets. Having considered the released energy associated with the phase change, the bulk of the vapour may then be regarded as a perfect gas for which the term \( \Delta h \) can be replaced by \( \Delta C_v \). Substituting this into equation (9), denoting \( (h_c - h_L) \) by L, regarding the term \( \frac{u_c^2}{2} \) small compared to L, neglecting \( W_L dL \), dividing throughout by \( MC_p T_c \), and rearranging results in [10]:
\[ \frac{dT_c}{T_c} = -\frac{1}{W} \frac{u_c^2}{C_p T_c} \frac{du_c}{u_c} + \frac{L}{C_p T_c} \frac{dW_L}{W} \]

Equations (3), (6), (8) and (10) can be solved for the four unknowns \( \frac{dT_c}{T_c}, \frac{dP}{P}, \frac{du_c}{u_c} \) and \( \frac{dW_L}{W} \), providing that \( \frac{dW_L}{W} \) are known as explained in reference [8].

III. NUCLEATION MODEL

For non-equilibrium flow calculations there must be a criterion for the onset of nucleation and the appearance of the second phase (liquid). The present model considers only homogenous nucleation in a pure substance and relies heavily on classical nucleation theory. The relevant nucleation theory is only briefly presented here.

The essence of the model is that in order for nucleation to occur in a flowing stream undergoing expansion, molecular clusters (the minute embryo of a liquid droplet) must overcome a free energy barrier, associated with the increase in surface-free-energy of the droplets, for the onset of phase change. As a substance is increasingly supercooled the chances of a molecular cluster moving over the free energy barrier increases.

If you are using Word, use either the Microsoft Equation Editor or the MathType add-on (http://www.mathtype.com) for equations in your paper (Insert | Object | Create New | Microsoft Equation or MathType Equation). “Float over text” should not be selected.

IV. DROPLET FORMATION

The change of Gibbs free energy for a mass \( m_r \) from a supercooled vapour at constant pressure and temperature that forms a liquid droplet at the same pressure and temperature,
can be calculated in four stages in the absence of magnetic and electrical fields:

\[ \Delta G = \Delta G_i + \Delta G_v + \Delta G_t + \Delta G_e \]

\( \Delta G_i \) (Isothermal expansion term)

\( \Delta G_v \approx 0 \) (Vapour phase change)

\( \Delta G_t \approx 0 \) (Isothermal compression Term)

\( \Delta G_e \) (Formation of droplet from bulk phase)

Based on the thermodynamic equilibrium, there is a minimum radius \( r^* \) (the critical radius) that must be attained in order to form a stable nucleus from supersaturated vapour. For this condition, the Gibbs’s free energy of formation of a critical cluster is denoted as \( \Delta G^* \). By differentiating equation (11) with respect to \( r \) the critical radius \( (r^*) \) and \( \Delta G^* \) are obtained.

\[ \Delta G^* = \frac{16\pi \rho \sigma^3}{\rho_i RT_c \ln p / p_i (T_c)} \]

\[ r^* = \frac{2\sigma}{\rho_i RT_c \ln[p / p_i (T_c)]} \]

Droplets with radius smaller than \( r^* \) have tendency to evaporate by losing their molecules and decreasing their Gibbs free energy. If the radius is greater than \( r^* \), the droplet will grow in the vapour phase.

V. NUCLEATION RATE EQUATION

Even within the body of a superheated vapour, molecular clusters are continually formed and disrupted by the statistical fluctuations. The statistically steady state population \( n_g \) of clusters containing \( g \) molecules is given by Boltzmann’s relation:

\[ n_g = n_i \exp \left[ \frac{\Delta G}{kT} \right] \]

where \( n_g \) and \( n_i \) are the numbers per unit volume of \( g \)-mers and monomers respectively. \( \Delta G \) is the free energy required to form a \( g \)-mers and \( K \) is the Boltzmann constant. If the rate of condensation and evaporation from a cluster are denoted by \( C \) and \( E \) respectively, then the equilibrium equation can be written as:

\[ n_gC_g = n_gE_{g+1} \]

In a supersaturated vapour, the processes of cluster formation and disruption are in a similar way, but if the clusters exceed the critical size they encounter a favorable \( \Delta G \) gradient and tend to grow. The steady state described by equation (15) is no longer applicable because the rates at which the clusters grow and decay are no longer balanced. To signify the difference, the symbol \( f_g \) is used to denote the concentration of \( g \)-mers under these conditions. The net rate per unit volume \( J_g \) at which \( g \)-mers grow to \((g+1)\)-mers is termed the nucleation current and can be expressed as:

\[ J_g = C_g f_g - E_{g+1} f_{g+1} \]

As given in Appendix c, for the constant nucleation current, it may be as follows:

\[ J_g \int \frac{dg}{C_g n_g} = \int \frac{dE_{g+1}}{E_{g+1}} = 1 \]

where \( C_g \) is proportional to \( r^2 \) and it is a slowly varying function. \( n_g \) may be written in terms of \( n_i \) using equation (14) and \( \Delta (G - G^*) \) may be expanded using Taylor series about \((g-g*)\).

With some assumptions as explained in appendix c, the equation (17) may be written as:

\[ J_g = \frac{C_g n_i \exp[-\Delta G^* / kT] \cdot \rho_i}{(2\pi kT)^{1/2} \zeta^{1/2}} \]

where

\[ \zeta = \frac{\partial^2 \Delta G}{\partial g^2} \]

The above reasoning in general, is true at low and high pressures. The only terms which can be affected by the virial coefficient in further developing the analysis, are \( \zeta \) and \( C_g \). \( \zeta \) is obtained by double differentiating of equation (11). To avoid the introduction of the virial coefficient, \( \zeta \) can be written in terms of density:

\[ \zeta = \frac{2}{9} \left( \frac{36\pi \sigma^2}{9} \right) \frac{J_g}{(g^*)^2} \]

\( C_g \) is evaluated from kinetic theory in terms of density:

\[ C_g = \frac{4\pi \sigma^2}{m} \left[ \frac{RT_c}{2\pi} \right] \frac{1}{\rho_i} \]

where \( m \) is the mass of a molecule and \( q \) is the condensation coefficient defined as the fraction of molecules colliding with the surface which are condensed. Combining equations (18), (19) and (20) the nucleation rate equation is given as:

\[ J_g = \frac{q}{m} \left[ \frac{2\sigma^2}{\pi} \right] \frac{1}{\rho_i} \frac{16\pi \sigma^3}{\rho_i RT_c \ln[p / p_i (T_c)]} \]

where

\[ m = \frac{4}{3} \frac{\pi \sigma^3}{\rho_i} \]
In the present investigation the nucleation theory adopted is the classical result subject to the refinements by Courtney and Kantrowitz [4] as follows:

\[
J_{nc} = \left( 1 + \frac{q G_s}{\alpha} \frac{RT_o^2}{2\pi} \right)^{4/3} \left( \frac{L}{RT_o} \right)^{1/2} \left( \frac{L}{2\pi} \right)^{1/2} \times \frac{1}{\rho_l (RT_o)} \exp \left[ -\frac{16\pi N^3}{3\rho_l (RT_o)} \ln \left( \frac{p}{P_l (T_l)} \right) \right] ^{1/3}
\]  

(22)

It should be noted that no universally applicable nucleation model is yet available for condensing flows; however the general form described here has been successfully used for steam at low pressures by a number of researchers [1]-[6]-[7]-[9].

VI. DROPLET GROWTH EQUATIONS

Once droplets are formed, they increase in size as vapour molecules condense on their surfaces. Released energy in condensation leads to a rise in the droplets temperature, and hence, the droplets become hotter than the surrounding vapour during the condensation. The growth is thus governed mainly by the mass flow towards a droplet and energy flux away from it. In a pure vapour, however, due to the release of a very high latent heat in the rapid condensation zone, the droplet growth is dominated by the thermal transfer rate. The energy conservation law can be formulated as:

\[
\frac{d}{dt} \left( \frac{4}{3} \pi r^3 \rho_l L \right) = \alpha 4 \pi r^2 (T_l - T_o)
\]

(23)

where \( \alpha \) is the coefficient of heat transfer from a droplet with radius \( r \) to the surrounding vapour. Therefore the droplet growth rate can be calculated if both \( \alpha \) and \( T_l \) are known:

\[
\frac{dr}{dt} = \frac{1}{\rho_l L} \alpha (T_l - T_o)
\]

(24)

Knudsen number, \( Kn \), plays a key role in the coefficient of heat transfer due to the wide range of droplet radii. Knudsen number is the ratio of the mean free path \( l \) of vapour molecules to the droplet diameter:

\[
Kn = \frac{l}{2r}
\]

(25)

For heat transfer coefficient, an empirical relation was presented in 1964 by Gyarmathy:

\[
\alpha_{\text{empirical}} = \frac{\lambda}{r(1 + 3.18Kn)}
\]

(26)

He also suggested the following equation for liquid temperature [4]:

\[
T_l = T_o + \left[ 1 - \frac{r}{R} \right] \left[ T_l(p) - T_o \right]
\]

(27)

Bakhtar and Zidi presented a semi-empirical relation for droplet's growth as explained in reference [11]:

\[
\frac{dr}{dt} = \frac{Kn}{Kn + 0.375} q_o \left( \frac{R}{\rho_l} \right)^{1/3} \times \left[ \rho_l \sqrt{\rho_l - \rho_l (T_l, r)} \right] ^{1/2}
\]

(28)

By numerical solution of equations (27) and (28) the droplet radius and temperature can be calculated [8].

In previous investigations aiming at predicting condensation, sometimes considerable differences have been observed between numerical values and experimental ones.

The uncertainties in making theoretical predictions of nucleation flows result from the uncertainties associated with the variation of surface tension at small droplet sizes, the value of the condensation coefficient and the equation of state for supercooled steam to calculate isentropic exponent that their importance will be elaborated below.

VII. IMPORTANCE OF SURFACE TENSION, CONDENSATION COEFFICIENT AND ISENTROPIC EXPONENT

SURFACE TENSION

Consideration of equation (22) for \( J \) shows that the surface free energy (surface tension) of the critical cluster \( \sigma \) appears raised to the third power in the exponential part of the expression. Small changes in \( \sigma \) clearly have a dramatic effect on the nucleation rate.

At the very high supersaturation ratios achieved in condensing nozzle flows, a critical droplet is composed of 10 – 50 molecules. It has been subject of much debate as to whether the surface free energies of such small clusters are well represented by flat-film values of surface tension. Based on the Gibbs theory of surface tension, liquid drop nucleation theory can be formally modified to include the effect of a radius – dependent surface free energy [13], but the problem comes in specifying exactly how \( \sigma \) varies with \( r \). Several theories have been proposed [3]. But there is no general agreement, even on the sign of the variation. However, because of the sensitivity of \( J \) to changes in \( \sigma \), it is unlikely that a satisfactory nucleation theory will be forthcoming until this problem is resolved.

CONDENSATION COEFFICIENT

The condensation coefficient \( q \) appears in the pre-exponential factor in the nucleation rate equation and so its effect is less drastic than that of the surface free energy. Early experiments indicated values around 0.02-0.03 [15], but it is now thought that these measurements were subject to large systematic errors and the general consensus is that \( q \) takes values close to one [14]. Such values are also consistent with results from Millikan’s classic oil drop experiment, where it
was estimated that about 90 percent of incident molecules suffered diffuse, as opposed to specular, reflection (implying that they had accommodated completely to the surface condition before re-emissio. Although most workers take q=1, it should be noted that all experimental evidence has been obtained with surfaces large on a molecular scale. For very small clusters that value of q is almost certainly much less than one (consider, for example, the extreme case of dimer formation from monomer-monomer collisions). [3]

Although the effect of condensation coefficient is not as marked as that of surface tension, it is still an important parameter that is directly proportional to the nucleation rate and also has a strong influence on droplet size by its inclusion in the droplet growth therefore, it’s exact value is of crucial importance for us.

**ISENTROPIC EXPONENT**

The equation of state and the associated properties are accurate in the superheated region down to the saturation line. In nozzle flows, however, much of the expansion takes place in the supercooled range. As yet there is no P-V-T data available to allow the equations to be checked in this region. Notwithstanding, the various formulae have been extrapolated to obtain supercooled properties but it must be emphatically stressed that the accuracy of these extrapolations are unknown and may possibly introduce large errors into the analysis. Of particular importance is the isentropic exponent k, which has a marked effect on the rate of expansion and hence on the nucleation point. Recently a few measurements of this variable in the supercooled range have been published, but they are too few in number to draw any useful conclusions. Thus the precise value of k is not known yet without which predicting the exact area of nucleation is not feasible.

**VIII. DESCRIBING THE REVERSE PROBLEM OR REVERSE METHOD**

Reverse problem is finding unknown parameters using the measured data gained through the process (discovering the cause through the effect); however due to the existence of error in measured values and criticality of the problem which will be explained in the next chapters it is not possible to use the direct and exact problem solving for the unknown parameter. Therefore it should be possible to present a decent description for reaching the answer. In this section the answer is described by examining the different methods for describing the problem.

In reverse problem error is $\tilde{e}$ the difference between measured output of the process is, $\tilde{T}^m$, and the output of the model on the spot, $\tilde{T}^e$ described as:

$$\tilde{e} = \tilde{T}^m - \tilde{T}^e \quad (29)$$

In order to minimize this error there are different ways to define the aimed function. One of the common ways is to use the squared error method. The aim in reverse problem is to minimize the sum of the squares:

$$S(\tilde{P}) = \tilde{e}^T \tilde{e} \quad (30)$$

The total of squared errors could change every effect of the errors by weight giving $W$ [16]

$$S(\tilde{P}) = [\tilde{T}^m - \tilde{T}^e]^T W [\tilde{T}^m - \tilde{T}^e] \quad (31)$$

$S$ is a function of the variable $\tilde{P}$. Employing derivative the optimized spot for function $S$ is determined which is as the following:

$$\frac{\partial S}{\partial \tilde{P}} = 0 \Rightarrow \nabla S(\tilde{P}) = 2 \left[ -\frac{\partial \tilde{T}^e}{\partial \tilde{P}} \right] W [\tilde{T}^m - \tilde{T}^e] = 0$$

or

$$\mathbf{X}^T W [\tilde{T}^m - \tilde{T}^e] = 0 \quad (32)$$

Here, the $\mathbf{X}$ sensitivity matrix is defined as the following in a way that it is not a function of unknown parameters for the reverse problems with linear behavior.

$$\mathbf{X} = \left[ \frac{\partial \tilde{T}(\tilde{P})}{\partial \tilde{P}} \right]$$

(33)

Regarding to the reserve problems with linear behavior including our problem the sensitivity matrix is dependent on $\tilde{P}$ vertex; therefore, solving the equation No. (29) Needs a trial and error method in which the trial and error method is introduced by linearizing the definite parameter vertex calculated by Taylor’s expansion around $\tilde{P}$ as the following:

$$\tilde{T}^e(\tilde{P}) = \tilde{T}^e(\tilde{P}^k) + \mathbf{X}^k (\tilde{P} - \tilde{P}^k) \quad (34)$$

In which the superscript “k” indicates the parameter amount at time step of “k”. Replacing equation No. (29) in equation No. (31) and rewriting the equation we will have:

$$\mathbf{X}^k W [\tilde{T}^m - \tilde{T}^e] = \mathbf{X}^k \Delta \tilde{P}$$

or

$$P^{k+1} = P^k + \left(\mathbf{X}^k \right)^T \mathbf{X}^k W [\tilde{T}^m - \tilde{T}^e(P^k)] \quad (35)$$

The introduced method in equation No. (35) is known as Gauss method. In fact, this method is an approximation for Newton – Raffin method. In order to have the possibility of solving the equation No. (35) the term $\mathbf{X}^k \tilde{X}^k$ must not be singular, in other words we will have:

$$\left| \mathbf{X}^k \tilde{X}^k \right| \neq 0 \quad (36)$$
The problems in which the above determinant becomes zero are known as critical problems and actually most of the reverse analysis problems are from this type.

**Methods to Select Parameters**

One of the most important methods was presented by Levenberg [17] which also has been called the least depreciated squares. This method based on statistical basis has been presented for the least depreciated squares. In this method term No. (30) is used as the following:

\[ S = (\tilde{T}^n - \tilde{T}^* )^\mathbb{T} W (\tilde{T}^m - \tilde{T}^* ) + \nu^k (\hat{P} - \tilde{P}^*)^\mathbb{T} \Omega^k (\hat{P} - \tilde{P}^*) \]  

or

\[ X^\mathbb{T} (\tilde{\theta}^n - \tilde{\theta}^* ) = (X^\mathbb{T} W + \nu^k \Omega^k) \Delta \hat{P} \]  

(37)

In this term \( \Omega^k \) is a diagonal matrix which reduces the change along the desired path restricting the deviation and when the related diagonal terms are bigger than diagonal terms \( X^\mathbb{T} WX \), causes reduction in vibration and instability. Levenberb showed that if adjustment coefficient is large at the beginning, \( S \) will reduce quickly and going on this coefficient must be reduced and that is because the answer of \( P^* \) could be incorrect and that is so gradients can find the real answer:

\[ \Omega^k \mathbb{=} \begin{bmatrix} C_{11} & 0 & \cdots & 0 \\ 0 & C_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & C_{LL} \end{bmatrix} \]  

(38)

In which:

\[ C_{ij} = W_{ij} X_{ij} X_{ij} \]  

(39)

In which tensorial summation has been used. This selection can cause the result of the method to be fixed under linear transition. In this condition the proper coefficient is obtained through the following term:

\[ \nu^k = \frac{\tilde{\theta}^n - \tilde{\theta}^*}{S^\mathbb{T} W X X^\mathbb{T} W (\tilde{\theta}^n - \tilde{\theta}^*)} \]  

(40)

Marquardt’s method is similar to Levenberg’s. In this method to change the adjustment coefficient equation No. (40) along with the following relation has been used:

\[ \nu^k = \frac{\nu_0}{(\alpha)^j} \]  

(41)

In which \( \nu_0 \) is a proper fixed number, and \( \alpha \) is any number larger than 1. This method like Levenberg’s causes equilibrium between the fastest decreasing inclination and Gaussian method. This method uses fastest decreasing inclination method during initial steps when matrix \( X^\mathbb{T} W X \) is critical and Gaussian method when getting close to the answer which causes the forenamed matrix to become benign. Generally, this method is more useful in contexts related to reverse problems. Therefore, Levenberg Marquardt’s method along with changing equation No. (32) functions as the following:

\[ P^{k+1} = P^{k} + \left( X^\mathbb{T} X + \nu^k \Omega^k \right)^{-1} \left( X^\mathbb{T} \left( T^n - T^\mathbb{c} (P^k) \right) \right) \]  

(42)

which \( \nu^k \) is a scalar value and also called depreciation parameter and \( \Omega^k \) is a diagonal matrix which is produced through the following relation:

\[ \Omega^k = diag\left( X^\mathbb{T} X \right) \]  

(43)

Introducing \( \nu^k \Omega^k \) to repetitive equation is done to depreciate the vibrations and instabilities caused by the problem criticality. Depreciative parameter at the beginning of simulation when the unknown parameter with the initial guess in introduced is usually large, hence due to the latter we no longer need to study the singularity of the term \( \left( X^\mathbb{T} X \right)^{-1} \).

**Convergence Criteria**

\[ \begin{align*}  
\| \Delta P^k \| &< \epsilon_1 \\
S &< \epsilon_2 \\
\frac{\left| S^{k-1} - S^k \right|}{S^2} &< \epsilon_3 
\end{align*} \]  

(44)

**Calculating the Sensitivity Matrix**

Calculating the sensitivity matrix is one of the great difficulties in nonlinear reverse problems. The component of “i” row and column “j” for a comprehensive problem according to the explanation is defined through the following relation:

\[ X_{ij} = \frac{\partial T^c}{\partial P_j} \]  

(45)

Which in this problem \( l = 1 \) and \( J = I_{max} \). Because the number of measured and calculated parameters on one spot has been considered, The following relation is used to calculate this component [18]:

\[ X_{ij} = \frac{T^c_i \left( P_i (1+\varepsilon)\right) - T^c_i (P_i)}{\varepsilon P_j} \]  

(46)

And thus an equation for correcting \( \hat{P} \) and a criteria for ending the reverse solving is gained.

**IX. CONCLUSION**

We change the source of two phase Code with using reverse method. For the initial guess we put Surface tension number equal zero in all the regime. In order to enhance the answers we have introduced the calculated laboratorial data
As it was stated before in case of lacking in laboratory results for the selected nozzle it could be possible to estimate the required pressure using the results of theoretical solution or laboratory results of analogous nozzle. This method is divided to Seven fundamental steps:

1. Solving direct problem by present estimation for \( P^k \) (unknown parameter) in order to reach direct solving parameter till the time of convergence.
2. Calculating \( S(P^k) \) using relation No. (26)
3. Calculating the sensitivity matrix using relation No. (43) and computing the depreciation term \( \Omega \) using relation No. (40) and the present amount for \( P^k \).
4. Solving the problem with the aid of Levenberg Marquardt’s method and calculating the new approximate amount \( P^{k+1} \) which is as the following:
\[
P^{k+1} = P^k + \Delta P^k
\]
5. Solving the direct problem using \( P^{k+1} \) in order to find the amount of \( T(P^{k+1}) \), then calculating \( S(P^{k+1}) \)
6. If \( S(P^{k+1}) \geq S(P^k) \), \( V^k \) 20 times multiplied
   If \( S(P^{k+1}) < S(P^k) \), \( V^k \) 0.5 times multiplied
7. Convergence criteria is to be checked, proceed to step (3) in case of convergence nonexistence.

APPENDIX

a) The virial coefficients of Vukalovich state equation
\[
B_i = - \frac{F}{GT} \phi_i + B_i - b \phi_i + 4b \phi_i^3; B_i = 32b \phi_i^2 \phi_i; B_i = 0; B_i = -4n \phi_i \phi_i
\]
Where
\[
\phi_i = \frac{CG}{T_i}; B_i = 1 - \frac{K}{T_i}
\]
And
\[
e = 63.2; b = 0.00085; C = 0.3900 \times 10^9; G = 47.053; K = 22.7;
n = 0.355 \times 10^{-1}; m_1 = 1.968; m_2 = 2.957
\]
\[
W_1 = \left(3+2m_1\right)/2; W_2 = \left(3m_2-4m_1\right)/2
\]

b) The thermodynamic properties
\[
h = p v - RT \left(\frac{1}{v} \frac{dp}{dv} \frac{1}{v^2} \frac{dp}{dv} + \frac{1}{v^3} \frac{dp}{dv} \right)
\]
\[
+ \left(1.111177T + 3.55878 \times 10^{-3}T^2 - \frac{6991.96}{T} + 2070.54\right)
\]
\[
s = R v + 0.30773 + 1.111177 \ln T + 7.11756 \times 10^{-7} T - \frac{3495.98}{T^2}
\]
\[
C_V = \frac{\partial}{\partial T} (h-p)v
\]
\[
C_p = C_V + \frac{\partial p}{\partial v}
\]
\[
R = 0.46151kJ/kgk
\]

c) Derivation of the nucleation rate equation
\[
n_g = \text{Number of cluster containing } g \text{ molecules per unit volume in equilibrium vapour.}
\]
\( f_g \): Number of cluster containing \( g \) molecules per unit volume in supercooled vapour.

\( C_g \): Rate of condensation. \( \left( g \to g + 1 \right) \)

\( E_g \): Rate of evaporation. \( \left( g \to g - 1 \right) \)

In the equilibrium condition, rate of condensation must be equivalent with rate of evaporation, so number of cluster containing \( g \) molecules must be constant.

\[
g - \frac{C_g}{E_g} \to g + 1 \quad \implies n_g C_g = n_g E_g \tag{c-1}
\]

In the supercooled vapour, there is a non-equilibrium condition so:

Growth rate of cluster containing \( g \) molecules = (Rate of condensation cluster containing \( g \) molecules) - (Rate of evaporation cluster containing \( g + 1 \) molecules):

\[
g - \frac{C_g}{E_g} \to g + 1 \\
g + 1 \to \frac{C_g}{E_g} \to g - 1 \\
\implies J_g = f_g C_g - f_g E_g \tag{c-2}
\]

Then growth rate of cluster containing \( g - 1 \) molecules is:

\[
g - 1 - \frac{C_g}{E_g} \to g - 1 \\
\implies J_{g-1} = f_{g-1} C_{g-1} - f_{g-1} E_{g-1} \tag{c-3}
\]

Therefore total growth rate of cluster containing \( g \) molecules is as follows:

\[
g - 1 - \frac{C_g}{E_g} \to g + 1 \\
g + 1 \to \frac{C_g}{E_g} \to g - 1 \\
\implies J_g = f_g C_g - f_g E_g \tag{c-4}
\]

Using equation (c-4) to obtain:

\[
\frac{\partial J_g}{\partial t} = \left( \frac{f_g C_g}{E_g} - f_g E_g \right) - \left( \frac{f_g C_g}{E_g} + f_g E_g \right) \\
\frac{\partial J_{g-1}}{\partial t} = \left( f_{g-1} C_{g-1} - f_{g-1} E_{g-1} \right) - \left( f_{g-1} C_{g-1} - f_{g-1} E_{g-1} \right) \\
\frac{\partial J_{g-1}}{\partial t} = J_{g-1} - J_g = \frac{J_g - J_{g-1}}{\Delta g} = \frac{\partial J_g}{\partial g} \quad \Delta g = 1
\]

Dividing equation (c-2) by \( n_g C_g \) to give:

\[
\frac{J_g}{n_g C_g} = \frac{f_g C_g}{n_g C_g} - \frac{f_g E_g}{n_g C_g} \tag{c-6}
\]

Substituting \( f_g E_g \) from equation (c-1) into equation (c-6):

\[
\frac{J_g}{n_g C_g} = \frac{f_g C_g}{n_g C_g} - \frac{f_g E_g}{n_g C_g} - \frac{\partial f_g}{\partial g} \frac{E_g}{n_g} \tag{c-7}
\]

Using equation (c-5) and (c-7) to get:

\[
\frac{\partial C_g}{\partial t} = \frac{\partial f_g}{\partial g} \left[ f_g C_g \right] = \frac{\partial f_g}{\partial g} \left[ f_g \right] \int \frac{C_g}{n_g} \int \frac{E_g}{n_g} \tag{c-8}
\]

To obtain an expression for \( J_g \) equation (c-8) is written for a series of cluster sizes in the range of \( 1 < g < g^* \) where \( g^* \) is much larger than \( g^* \).

The assumptions for obtaining equation (18) are as follows:

a) \( C_g \) is taken out of the integral and is given it a mean value say as \( C_{g^*} \), then the integral is carried out.

b) With very little loss of accuracy, the limits of integral is changed from \(-\infty \) to \(+\infty \).

REFERENCES


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