Integrating Finite Element Based Heat Transfer Analysis with Multivariate Optimization for Efficient Weld Pool Modeling

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Measurement of weld thermal cycle and peak temperature is a difficult task in fusion welding due to high peak temperature and rapid thermal cycle. Numerical modeling of heat transfer process in fusion welding provides a useful tool for the prediction of the weld pool shape and thermal cycles. However, the reliability of the predictions greatly depends on the accuracy of the input parameters provided to such models. In the case of laser beam welding, the absorptivity represents an important variable that defines the actual heat input for a given power while the value of absorptivity rarely known a-priori with confidence. The present work provides a novel framework where the unknown value of the absorptivity is obtained using an inverse approach by integrating finite element based heat transfer simulation and multivariate optimization procedure. The heat transfer simulation predicts the weld pool dimensions for known welding conditions and assigned values of absorptivity. The optimization algorithm tracks the error in the prediction, its sensitivity with small change in absorptivity, and finally yields the optimum value of absorptivity iteratively. Eight known welding conditions and corresponding weld pool measurements were utilized in this work. It is experienced that the optimum value of absorptivity remains nearly same irrespective of the number of known measurements used for the optimization process thereby indicating the robustness of the inverse approach.

KEY WORDS: laser spot welding; modeling; finite element method; heat conduction; parameter optimization.
the weld pool. The optimization algorithm then minimizes the error between the predicted and the experimentally observed penetrations and the weld widths by considering the sensitivity of the computed weld pool dimensions with respect to the absorptivity. The sensitivity terms are calculated by running the heat transfer model several times for each measurement considering small changes in the absorptivity. Two well tested non-linear optimization algorithms are followed in the present work—Levenberg Marquardt method and Conjugate Gradient Technique. The optimum value of the absorptivity is found out using both the optimization algorithms separately using a number of initial guess values to test the robustness of the integrated procedure. It has been observed that the final optimum value of absorptivity remains unchanged irrespective of the initial guess and the optimization method.

The work presented in this manuscript represents an improvement over the previous reverse modeling work in welding reported in the literature. First, unlike the previous efforts, a finite element based numerical heat transfer model considering non-linear material properties and effect of phase change is used to compute the weld pool geometry. Secondly, two well-tested nonlinear multivariate optimization techniques have been used for the estimation of the optimum value of absorptivity. Eight sets of experimentally measured weld pool widths and penetrations, presented in Table 1, are used for optimizing the value of absorptivity. The welds are made with a high power diode laser having a laser spot radius of 0.5 mm on a 2.0 mm thick C–Mn Steel Sheet (Table 2). The optimization exercise has been carried out using all sets of measured weld pool dimensions and also with a number of smaller subsets of the total number of measurements. The optimized value of the absorptivity remained identical in all cases manifesting the robustness of the present integrated modeling procedure.

2. Heat Transfer Simulation

Considering the radial symmetry of the laser beam applied to a substrate, a two-dimensional, axisymmetric, transient heat conduction analysis is conducted in the present work based on finite element method (Fig. 1). The numerical model considers latent heat of transformations and temperature dependent thermo physical properties. The governing heat conduction equation in cylindrical coordinates is given as:

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \frac{\partial T}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + \dot{Q} = -\rho c \frac{\partial T}{\partial t} \\
\text{..................................................(1)}
\]

where, \( r \) and \( z \) refer to radial and axial directions, \( k \), \( \rho \), and \( c \) respectively to thermal conductivity, density, and specific heat of material, \( T \) and \( t \) refer to temperature and time variables. \( \dot{Q} \) depicts the rate of internal heat generation per unit volume. The generalized boundary condition is represented as:

\[
k_n \frac{\partial T}{\partial n} + q + h(T - T_a) + \sigma \varepsilon (T^4 - T_a^4) = 0 \quad \text{..........................(2)}
\]

Table 1. Measured weld dimensions and welding parameters.\(^{1-3}\)

| Data set index | Laser power (W) | On-time (s) | Weld width (mm) | Weld penetration (mm) |
|---------------|----------------|-------------|-----------------|-----------------------|
| 1             | 1400           | 0.150       | 1.43            | 0.43                  |
| 2             | 1400           | 0.650       | 2.50            | 1.14                  |
| 3             | 2240           | 0.150       | 2.53            | 1.26                  |
| 4             | 2240           | 0.165       | 2.53            | 1.53                  |
| 5             | 2240           | 0.180       | 2.70            | 1.73                  |
| 6             | 2240           | 0.195       | 2.70            | 1.80                  |
| 7             | 2240           | 0.210       | 2.80            | 2.00                  |
| 8             | 2240           | 0.225       | 2.80            | 2.00                  |

Table 2. Chemical composition (in wt%) C–Mn steel used for laser spot welding.\(^{13}\)

| C   | Cr   | Mo | V   | Mn  | Si | Ni |
|-----|------|----|-----|-----|----|----|
| 0.07| 0.04 | < 0.01 | < 0.01 | 0.92 | 0.10 | 0.02 |

where, \( n \) refers to the direction normal to surface; \( k_n \), \( h \), \( \varepsilon \), \( \sigma \) and \( T_a \) refer respectively to thermal conductivity normal to surface, surface heat transfer coefficient, emissivity, Stefan–Boltzmann constant and the ambient temperature. The third and fourth terms in the left hand side of Eq. (2) respectively refer to convective and radiative heat loss from the surface of the substrate. The term \( q \) stands for the imposed heat flux onto the surface due to the laser beam. Since the process is transient in nature, an additional boundary condition is needed at time \( t=0 \) as:

\[ T(r, z, t)=0 \quad \text{at} \quad t=0 \quad \text{..........................(3)} \]

To avoid the non-linearity due to the term corresponding to the radiative heat loss a lumped heat transfer coefficient \( h \) is used in combining the convective and radiative heat loss and is given as:\(^{2,3}\)

\[ h=2.4 \cdot 10^{-3} \cdot \varepsilon \cdot T^{1.61} \quad \text{..........................(4)} \]

The applied heat flux \( q \) on the top surface of the substrate due to the laser beam is assumed to follow Gaussian distribution that can be mathematically expressed as:
\[ q(r) = \frac{P \eta d}{\pi r^2_{\text{eff}}} \exp\left( -\frac{dr^2}{r^2_{\text{eff}}} \right) \] ...................(5)

where, \( P \), \( \eta \), \( r_{\text{eff}} \), and \( d \) refer respectively to the beam power, absorptivity, effective radius of beam on the top surface of the substrate and beam distribution coefficient. In Eq. (5), the value of absorptivity is very important since it defines the actual power input to the substrate. Since the value of absorptivity depends on substrate surface, peak temperature, etc. in real time, its value cannot be pre-defined with confidence. It is considered to be an unknown parameter in the present work.

The governing equation along with the boundary condition has been discretized first in spatial coordinate system using four node isoparametric element\(^{30}\) and next in time domain using linear variation of temperatures within a small time interval following Galerkin’s Weighted residue technique\(^{30}\) The final matrix equation to be solved is expressed as \(^{30}\):

\[
\left( \frac{2}{3} \left[ H \right] + \frac{1}{\Delta t} \left[ S \right] \right) \left[ T \right]_{n+1} + \left( \frac{1}{3} \left[ H \right] - \frac{1}{\Delta t} \left[ S \right] \right) \left[ T \right]_n + \frac{2}{(\Delta t)^2} \int_0^{\Delta t} \{ f \} dt = 0 \] ...................(6)

where \( \{ T \}_{n+1} \) and \( \{ T \}_n \) refer to the temperature variables respectively after \((n+1)\)th and \(n\)th iterations, and \( \Delta t \) depicts the time interval between two successive iterations. The general expressions of various terms in Eq. (6) are given as \(^{30}\):

\[
h_{ij} = \int \int_{v'} \left( k \frac{\partial N_i}{\partial r} \frac{\partial N_j}{\partial r} + k \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) 2 \pi r dr dz \]

\[
+ \int h N_i N_j 2 \pi r dl \] ...................(7)

\[
s_{ij} = \int \int_{v'} N_i \rho c N_j 2 \pi r dr dz \] ...................(8)

\[
f_i = \int \int_{v'} \left( N_i \partial T / \partial r \right) 2 \pi r dr dz + \int h N_i T 2 \pi r dl + \int q N_i 2 \pi r dl \] .............................(9)

In Eqs. (7)-(9), \( N_i \) and \( N_j \) refer to the elemental shape functions corresponding to the \(i\)th and \(j\)th nodes, and the superscript \( e \) refers elements used to discretize the substrate geometry. The first term in Eq. (9) is zero here since no internal heat generation is present here. The second and third terms in Eq. (9) correspond respectively to surface heat loss due to convection and input heat flux due to the laser beam applied on the top surface of the substrate (Fig.1). Figure 2 presents the temperature dependent material properties that have been considered in the numerical calculations. Furthermore, the latent heat is considered as an appropriate increase or decrease in specific heat during melting or solidification respectively\(^{30}\).

3. Optimization Procedure

The optimization process using LM and CG methods involves the finding the minimum of an objective function \( O(f) \) that depicts the error between the estimated and the corresponding measured values of one or more dependent variables obtained from \( M \) number of observations\(^{22,23,31}\). In the present work, the objective function \( O(f) \) is defined using weld penetration and weld width as two dependent variables as:

\[
O(f) = \sum_{m=1}^{M} \left[ \frac{p^m_{\text{obs}} - p^m_{\text{cal}}}{p^m_{\text{obs}}} \right]^2 + \sum_{m=1}^{M} \left[ \frac{w^m_{\text{obs}} - w^m_{\text{cal}}}{w^m_{\text{obs}}} \right]^2 \\
= \sum_{m=1}^{M} \left[ p^m_{\text{obs}} - p^m_{\text{cal}} \right]^2 + \sum_{m=1}^{M} \left[ w^m_{\text{obs}} - w^m_{\text{cal}} \right]^2 \] .............................(10)

where \( p^m_{\text{obs}} \) and \( w^m_{\text{obs}} \) are the penetration and the width of the weld pool computed by the numerical heat transfer model, respectively, \( p^m_{\text{cal}} \) and \( w^m_{\text{cal}} \) are the corresponding measurements at similar welding conditions, and \( p^m_{\text{obs}} \) and \( w^m_{\text{obs}} \) are non-dimensional and indicate the extent of over- or under-prediction of penetration and weld width, respectively. \( M \) corresponds to the number of known sets of measured values of weld width and weld penetration for which the welding conditions are also known. In Eq. (10), \( f \) stands for the independent variable which is unknown and eventually, \( O(f) \) is a function of \( f \). In the present work, \( f \) corresponds to the unknown absorptivity, \( \eta \).

Assuming that \( O(f) \) is continuous and has a minimum value, the LM method tries to obtain the optimum values of \( \eta \) by minimizing \( O(f) \) with respect to it i.e. Eq. (10) is differentiated with respect to \( \eta \) and made equal to zero as:

\[
\frac{\partial O(f)}{\partial \eta} = \sum_{m=1}^{M} \left( \frac{p^m_{\text{cal}} - p^m_{\text{obs}}}{p^m_{\text{obs}}} \right) \frac{\partial p^m_{\text{cal}}}{\partial \eta} + \sum_{m=1}^{M} \left( \frac{w^m_{\text{cal}} - w^m_{\text{obs}}}{w^m_{\text{obs}}} \right) \frac{\partial w^m_{\text{cal}}}{\partial \eta} \\
= 2 \sum_{m=1}^{M} \left( p^m_{\text{cal}} - p^m_{\text{obs}} \right) \frac{\partial p^m_{\text{cal}}}{\partial \eta} + \sum_{m=1}^{M} \left( w^m_{\text{cal}} - w^m_{\text{obs}} \right) \frac{\partial w^m_{\text{cal}}}{\partial \eta} \] .............................(11)

The variables \( p^m_{\text{cal}} \) and \( w^m_{\text{cal}} \) in Eq. (10) are obtained from the numerical heat transfer model for a certain value of \( \eta \). The partial derivatives in Eq. (11) are termed as the sensitivity of the computed weld width and penetration with respect to \( \eta \) and these are calculated numerically as:
The dependence of the computed weld dimensions, \( p_m^* \) and \( w_m^* \), and in turn, of \( p_m^* \) and \( w_m^* \) on \( \eta \) can be explained as follows. As the value of \( \eta \) increases, the rate of actual heat input from the laser beam to the substrate is enhanced for the same power (Eq. (5)). An increase in the rate of actual heat input results in increased peak temperature and greater temperature gradient that, in turn, enhances the conduction heat transfer in both the radial and downward directions. Thus, an increase in the value of \( \eta \) readily improves \( p_m^* \) and \( w_m^* \), and in turn, of \( p_m^* \) and \( w_m^* \). Owing to the smaller substrate thickness compared to its radial dimension, \( p_m^* \) equals to the substrate thickness at a certain higher value of \( \eta \) and further increase in \( p_m^* \) and thus in \( p_m^* \) becomes not feasible. On the contrary, enhancement in the computed values of \( w_m^* \) with increase in the value of \( \eta \) is continually competed with the convective heat dissipation through the bulk of the substrate. It is realized that an increase in \( w_m^* \) effectively increases the size of the solid–liquid boundary of the weld pool thereby allowing larger area for convective heat transfer through the solid substrate. Thus, as the computed values of \( w_m^* \) become sufficiently greater than the spot diameter of the incident beam, the influence of the convective heat dissipation through bulk substrate becomes dominant and further enhancement in \( w_m^* \) slows down. This is observed for almost all the data sets in Table 1. An artifact of the present numerical heat transfer model is that the convective heat transport in weld pool is not accommodated. Nevertheless, the main objective of the present paper is to
demonstrate a novel approach how appropriate multivariate optimization methods can help in identifying uncertain parameters that are required for weld pool modeling. As convection heat transfer based weld pool models involves even more unknown parameters, the same approach can be useful too.\textsuperscript{23,24}

The dimensionless squared error in the computed values of penetration and weld width, i.e. \((p^*_m-1)^2\) and \((w^*_m-1)^2\), are summed up considering the data sets \#3 to \#8 (in Table 1) and plotted separately as a function of assumed \(\eta\) in Fig. 5. The resultant value of \(O(f)\) (following Eq. (10)) at each value of \(\eta\) is also plotted in Fig. 5. It can be observed in Fig. 5 that the value of \((p^*_m-1)^2\) for data sets \#3 to \#8 (in Table 1) decreases steadily as the value of \(\eta\) increases from 0.2 to 0.32 (approximately) and thereafter shows a slow increasing trend. On the contrary, the value of \((w^*_m-1)^2\) as around 0.31 for all the four initial guessed values. Figure 6(b) depicts that the minimum achievable value of \(O(f)\) is around 0.9 and it cannot be reduced further. The number of iterations required to reach the minimum attainable value of \(O(f)\) with the initial guessed value of \(\eta\) as 0.2, 0.3, 0.4 and 0.5 are respectively eight, four and two. The fact that all the initial guessed values has led to the same optimum value of \(\eta\) possibly proves that the heat transfer model should be able to capture the optimized value of \(\eta\) around 0.32 when data sets \#3 to \#8 (in Table 1) would be considered.

To calculate the optimized values of efficiency following the both LM and CG methods, an initial guessed value is necessary for parameter \(\eta\) considered unknown here. Figs. 6(a) and 6(b) respectively show the progress of \(\eta\) and \(O(f)\) with the number of iterations using four different initial guess values of \(\eta\) following the LM method of optimization. All the eight data sets (in Table 1) are considered in these calculations. Figure 6(a) shows that the optimum value of \(\eta\) as around 0.31 for all the four initial guessed values.

Similarly, Figs. 7(a) and 7(b) respectively show the progress of \(\eta\) and \(O(f)\) with the number of iterations using four different initial guess values of \(\eta\) following the CG method of optimization. All the eight data sets (in Table 1) are considered in these calculations. Figures 7(a) and 7(b) respectively show the optimum achievable value of \(\eta\) as 0.31 and the minimum attainable value of \(O(f)\) as approximately 0.9 for all the initially guessed values of \(\eta\). The
number of iterations required to reach the minimum attainable value of \( O(f) \) with the initial guessed value of \( \eta \) as 0.2, 0.3, 0.4 and 0.5 are respectively eight, four, four and two following the CG method of optimizing calculations. As in LM method, all the four initial guessed values has led to the same optimum value of \( \eta \) also in CG method. However, the number of iterations required to reach the optimum value of \( \eta \) are sometimes different between LM and CG methods for some initial guessed values. Since one optimizing iteration requires the numerical heat transfer analysis to run for \((M*N/M)\) times (where \(M\)=number of measurements and \(N\)=number of unknowns), any reduction in the number of iterations is significant.

A comparison between the experimentally measure weld pool and the corresponding computed weld fusion zone using the optimized value of absorptivity is represented in Fig. 8 for laser power of 1400 W and on-time of 0.15 s. The computed weld pool boundary is represented by the isothermal contour of 1773 K while a white line is marked in the experimentally measured fusion zone. A sufficiently satisfactory agreement between the measured and computed fusion zone can be realized in Fig. 8. The discrepancy in the weld width might have been caused due to the neglect of convective heat transport in the weld pool in the numerical model. Furthermore, the numerical calculation is done for all the eight data sets (Table 1) using the optimum value of absorptivity to obtain the computed values of penetration and weld width. Figure 9 shows the under- or over-prediction in weld pool dimensions for all the data sets where the computations are performed using the optimum value of \( \eta \) (~0.31). A fair agreement can be observed with respect to the values of the predicted penetration in all cases. As envisaged, the predicted weld pool width remains slightly under-predicted in all the cases. As a part of the optimization exercise, similar calculations have been done using various combinations of smaller number of data sets from Table 1. The optimized value of absorptivity has remained unchanged.

It is thus realized that the multivariate optimization methods such as LM and CG methods can be effectively integrated to conventional numerical heat transfer models of weld pool to identify the optimum value of an unknown parameter required for such modeling. Once such absorptivity or similar unknown modeling parameters are identified, a further application of such integrated model can be to identify the suitable set of welding process parameters for a targeted weld pool dimensions. Such integrated approach is far more convenient than neural network based model for estimating suitable process parameters for two reasons. Firstly, a very few experimentally measured values of weld dimensions and corresponding welding conditions are required in comparison to the large database that is essential for training of a neural network based model. Secondly, the

Fig. 7. Results of optimization calculation with all eight measurements using CG method [(a) \( \eta \) and (b) \( O(f) \) as a function of iterations].

Fig. 8. Comparison of experimental (left) and computed (right) fusion zone at laser power of 1400 W and on-time of 0.15 s. The computed weld pool shape is obtained considering the optimum value of absorptivity \( \eta \) as 0.31. The computed temperature values shown in the right figure are in °C.

Fig. 9. Comparison of measured weld dimensions and corresponding computed values in dimensionless form. Computed values are obtained for all eight data sets using optimum value of absorptivity \( \eta \) as 0.31.
integrated model presented here inherently links the input process parameters with the weld pool dimensions through fundamental relations of heat transfer. It is obvious that the incorporation of convective heat transport will further enhance the reliability of the numerical modeling results. The intensive computational work needed to determine the uncertain parameters results in enhanced reliability of the numerical modeling of heat transfer and fluid flow in the weld pool.

5. Conclusions

The traditional numerical heat transfer calculation in the weld pool is integrated with well-established, gradient-based, multivariate optimization techniques to inherently identify the unknown parameters required for modeling. The optimum value of absorptivity for laser spot welding that is obtained in the present work following the integrated model agrees well with such values reported in the previous literatures. Although the integrated approach enhances the volume of numerical calculations, such approach is possibly worth exploring for two reasons. Firstly, the integrated model presented here depicts a systematic approach to make numerical process models more reliable instead of trial-and-error numerical experiments with random choice of unknown modeling parameters so as to match the predicted values of weld pool dimensions with experimental measurements. Secondly, it is quite possible to use the integrated model for a-priori designing of welding process even by design experts not so familiar with numerical modeling of weld pool. This can pave the way for enhanced use of numerical heat transfer models in actual design process instead of their confinement more in academic research.

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Appendix 1.

In order to explain the basic concept of the LM method, an optimization problem involving the unknown parameter, \( \eta \), and one dependent variable, \( p_n^* \), measured under three welding conditions is explained first. Eq. (13) can be written for \( \eta \) as:

\[
\sum_{m=1}^{3} \left[ (p_{m}^{*} - 1) \frac{\partial p_{m}^{*}}{\partial \eta} \right] = 0 \quad \text{..............(A-1)}
\]

The value of the unknown, \( \eta \), cannot be directly obtained from Eq. (A.1) since it does not appear explicitly in this equation. So, the dependent variable, \( p_{n}^{*} \), is expanded using the Taylor’s series as:

\[
(p_{n}^{*})_{k+1} = (p_{n}^{*})_{k} + \frac{\partial (p_{n}^{*})_{k}}{\partial \eta} \Delta \eta_{k} \quad \text{..............(A-2)}
\]

where \((p_{n}^{*})_{k}\) and \((p_{n}^{*})_{k+1}\) are the values of \( p_{n}^{*} \) after \( k \text{th} \) and \((k+1)\text{th}\) iterations. \( \Delta \eta_{k} \) is the unknown increment corresponding to \( \eta \) as:

\[
\eta_{k+1} = \eta_{k} + \Delta \eta_{k} \quad \text{..............(A-3)}
\]

and \( \eta_{k+1} \) corresponds to the unknown value of \( \eta \) after \((k+1)\text{th}\) iteration. Except \( \Delta \eta_{k} \), all other terms on the right hand side of Eq. (A.2) are known. To solve for \( \Delta \eta_{k} \), Eq. (A.1) is rewritten replacing \( p_{n}^{*} \) by \( (p_{n}^{*})_{k+1} \) as:

\[
\sum_{m=1}^{3} \left[ (p_{m}^{*})_{k+1} - 1 \right] \left( \frac{\partial p_{m}^{*}}{\partial \eta} \right)_{k} = 0 \quad \text{..............(A-4)}
\]

However, \( p_{n}^{*} \) equals to \( p_{n}^{*}/p_{n}^{obs} \) and although \( p_{n}^{obs} \) is a known measured value, \( p_{n}^{*} \) is computed using the finite element based heat transfer calculation for a set of \( \eta \) and other known parameters. Since \( \eta_{k+1} \) is unknown, \( p_{n}^{*} \) after \((k+1)\text{th}\) iteration is also unknown and thus, \((p_{n}^{*})_{k+1}\) is not known. So, substituting Eq. (A.2) in Eq. (A.4), the latter can be rewritten as:
Neglecting higher order differentials e.g. \( \frac{\partial((\partial p_n^*)^i/\partial \eta)}{\partial \eta} \). Eq. (A-5) is further simplified as:

\[
\sum_{n=1}^{3} \left[ \left( \frac{\partial(p_n^*)^k}{\partial \eta} \right) \eta^i - 1 \right] \frac{\partial(p_n^*)^k}{\partial \eta} = 0 \tag{A-6}
\]

Equation. (A-6) can be rearranged as:

\[
\Delta \eta^i = -\sum_{n=1}^{3} \left[ \frac{\partial(p_n^*)^k}{\partial \eta} \right] \left( \frac{(p_n^*)^k - 1}{\eta} \right) \sum_{n=1}^{3} \left[ \frac{\partial(p_n^*)^k}{\partial \eta} \frac{\partial(p_n^*)^k}{\partial \eta} \right] \tag{A-7}
\]

The solution of \( \Delta \eta^i \) is used next to obtain \( \eta^{i+1} \) using Eq. (A-3) that is employed to compute the value of \( p_n^* \) after \((k+1)\) iteration using the numerical heat transfer model. Next, \( O(f)^{k+1} \) is calculated as:

\[
O(f)^{k+1} = \sum_{n=1}^{3} \left( \frac{\partial(w_n^*)^k}{\partial \eta} \right) \left( \frac{(w_n^*)^k - 1}{\eta} \right) \tag{A-8}
\]

The value of \( \eta \) is considered to be optimum when the calculated value of \( O(f)^{k+1} \) is smaller than a predefined small number. For the two dependent variables, \( p_n^* \) and \( w_n^* \), Eq. (A-7) is modified as:

\[
\Delta \eta^i = -\sum_{n=1}^{3} \left[ \frac{\partial(p_n^*)^k}{\partial \eta} \right] \left( \frac{(p_n^*)^k - 1}{\eta} \right) + \frac{\partial(w_n^*)^k}{\partial \eta} \left( \frac{(w_n^*)^k - 1}{\eta} \right) \tag{A-9}
\]

However, the sensitivity terms such as \( \frac{\partial(p_n^*)^k}{\partial \eta} \) or \( \frac{\partial(w_n^*)^k}{\partial \eta} \) in Eq. (A-9) may be very small as the value of the unknown parameter, \( \eta \), moves close to the optimum.\(^{31}\)

To avoid the resultant numerical instability in solving Eq. (A-9), the same is further modified following LM method as:

\[
\Delta \eta^i = -\sum_{n=1}^{3} \left[ \frac{\partial(p_n^*)^k}{\partial \eta} \right] \left( \frac{(p_n^*)^k - 1}{\eta} \right) + \frac{\partial(w_n^*)^k}{\partial \eta} \left( \frac{(w_n^*)^k - 1}{\eta} \right) + \lambda \tag{A-10}
\]

where \( \lambda \) is a scalar quantity, which ensures that the denominator of Eq. (A.10) will remain non-zero. The value of \( \lambda \) is usually increased or decreased by a factor of ten as the value of the objective function in subsequent iterations increases or decreases. This, in effect, ensures the reduction.

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![Fig. 10. Flow chart of the complete model using LM method of optimization.](image)

![Fig. 11. Flow chart of the complete model using CG method of optimization.](image)
or enhancement in step size as the solution respectively tends to diverge or converge. **Figure 10** presents the flow-chart of the complete procedure using LM method.

**Appendix 2.**
Substituting Eq. (14) in Eq. (15), the latter can be rewritten as:

\[
\frac{\partial O(\eta^k - \beta^k d^k)}{\partial \beta^k} = 0; \quad \beta^k \geq 0 \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots 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