**How to Use LS-OPT for Parameter Estimation – hot stamping and quenching applications**

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The "direct" heat transfer problem is one in which material properties and boundary conditions are specified, and LS-DYNA [1] is used to calculate the temperature response of the nodes in the mesh. The "inverse" heat transfer problem is one in which the temperature response of a node point in the mesh (e.g., a surface node) is specified from experimental measurements, and the objective is to calculate material properties and boundary conditions that cause this temperature response. This paper describes how to use LS-OPT [2] to solve the "inverse" heat transfer problem. Applications include:

- calculating material parameters for austenite-to-martensite phase change kinetics – fitting material properties to experimental data
- calculating contact heat transfer coefficients as a function of temperature and pressure during hot stamping – fitting a function to experimental data
- calculating boiling heat transfer coefficients for quenching in liquids – fitting a load curve to experimental data

## MAT_UHS_STEEL Phase Change Kinetics

This section describes how to use LS-OPT to calculate material properties for MAT_UHS_STEEL (MAT_244). The methodology shows how to calculate the phase transformation activation energies by matching numerical results with experimental measurements of Vickers hardness. The ultra high strength steel material model requires specification of the ferrite ($Q_f$), pearlite ($Q_p$) and bainite ($Q_b$) activation energies used in the phase change kinetic equations:

$$\frac{dx_f}{dt} = f(x_f)f(G)f(T)exp\left(-\frac{Q_f}{T}\right)$$

$$\frac{dx_p}{dt} = f(x_p)f(G)f(T)exp\left(-\frac{Q_p}{T}\right)$$

$$\frac{dx_b}{dt} = f(x_b)f(G)f(T)exp\left(-\frac{Q_b}{T}\right)$$

The functions $f(x_f)$, $f(x_p)$, and $f(x_b)$ account for the effect of the current fraction formed on the reaction rate. The function $f(G)$ accounts for the grain size and $f(T)$ accounts for undercooling. The material hardness is a function of the individual phase fractions ($x_i$) and hardness ($H_i$)

$$H = x_f H_f + x_p H_p + x_b H_b + x_a H_a$$

Where the phase hardness values, $H_i$ , are a function of the cooling rate at 700C.

$$H_i = C_i ln\left(\frac{dT}{dt}\right)_{T=700C}$$

Table 1 presents experimental data of Vickers hardness versus cooling rate [3] for USIBOR 1500P with an ASTM grain size of 6.8. The third column in Table 1 is calculated results after the optimization. Each experimental hardness value in Table 1 is for a different cooling rate. The LS-DYNA model consists of 10 separate parts, one for each cooling rate. Each part is a single shell element. A minimum of 3 parts are required to obtain a global minimum because there are 3 parameters to be optimized, $Q_f$, $Q_p$, and $Q_b$. Since the data was available, 2 extra parts were added to span the experimental data set and obtain a better answer. The 5 points selected for the parameter optimization are shaded in Table 1.

Table 1. Shown in the table are the experimental and calculated hardness values versus cooling rate. Values in the shaded boxes were used in the optimization response functions

| Cooling rate [C/sec] | Experimental Vickers hardness [ref. 3] | Calculated Vickers Hardness |
|---|---|---|
| 1 | 181 | 181 |
| 5 | 244 | 244 |
| 10 | 331 | 331 |
| 12.5 | 375 | 372 |
| 15.0 | 407 | 406 |
| 17.5 | 435 | 429 |
| 20 | 451 | 443 |
| 25 | 458 | 457 |
| 30 | 464 | 465 |
| 40 | 469 | 472 |

The optimization problem is addressed by minimizing the relative error in Vickers hardness. LS-DYNA calculates Vickers hardness and prints it out as element history variable #6 in the d3plot file. For the first data point in Table 1, the response function is

ResExp1=abs(Final(“hv61(t)-181)/181.

Where,

hv61(t) = d3plot element time history of Vickers hardness (i.e., history variable 6)

Final = lsopt script to use the final value

abs = lsopt script to take the absolute value

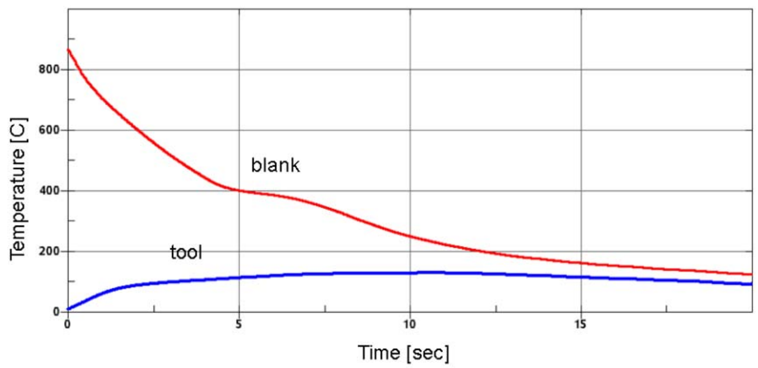
The remaining 4 response functions and other LS-OPT input parameters are shown in Table 2. The results are $Q_f$ = 11335, $Q_p$ = 16431, and $Q_b$ = 15035. An alternate approach is to define a composite mean squared error response function as demonstrated by the “System Parameter Identification” problem in the LS-OPT training manual [4].

| Table 2. LSOPT input parameters | |
|---|---|
| Strategy | SRSM – sequential with domain reduction |
| Variables | QR2(start, min, max) = (13022, 10000, 15000)<br>QR3(start, min, max) = (15570, 14000, 18000)<br>QR4(start, min, max) = (15287, 14000, 18000) |
| Sampling | Polynomial, linear, D-Optimal |
| Histories | hv61(t) = History variable 6 for part 1 with cooling rate 1<br>hv62(t) = History variable 6 for part 2 with cooling rate 5<br>hv63(t) = History variable 6 for part 3 with cooling rate 10<br>hv64(t) = History variable 6 for part 4 with cooling rate 15<br>hv65(t) = History variable 6 for part 5 with cooling rate 30 |
| Response | ResExp1 = abs(Final(“hv61(t)-181)/181<br>ResExp2 = abs(Final(“hv62(t)-244)/244<br>ResExp3 = abs(Final(“hv63(t)-331)/331<br>ResExp4 = abs(Final(“hv64(t)-407)/407<br>ResExp5 = abs(Final(“hv65(t)-465)/465 |
| Objective | ResExp1 = 1<br>ResExp2 = 1<br>ResExp3 = 1<br>ResExp4 = 1<br>ResExp5 = 1 |
| Constraints | None |
| Algorithm | LFOP |
| Run | 20 iterations |

**Contact Heat Transfer Coefficients**

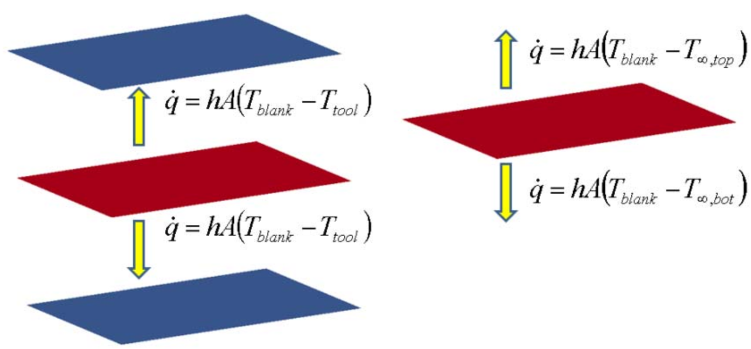
This section describes how to use LS-OPT to calculate hot stamping tool-to-blank contact heat transfer coefficients as a function of interface pressure. The described methodology shows how to fit a function (e.g., *DEFINE_FUNCTION) to experimental data. Experimental data [5] consists of temperature-time histories for thermocouples mounted below the surface of the blank, top tool, and bottom tool at several applied pressures. Data was recorded for P=0, 20MPa, and 30MPa. Figure 1 shows experimental data for P=0.

Figure 1. Experimental temperature versus time for P=0.




The contact heat flux from the hot blank to the cooler tools is calculated by $\dot{q} = hA\left(T_{blank} - T_{tool}\right)$ as shown in figure 2. This is similar to the equation used for convection boundary conditions, $\dot{q} = hA\left(T_{blank} - T_{\infty}\right)$. Therefore, instead of defining the model as a coupled thermal-stress problem, it can be defined as a thermal only problem using a convection boundary condition. $T_{\infty}$ is specified for the top and bottom blank surfaces using the experimental tool temperature data. By this methodology, we avoid the numerical application of a pressure boundary condition on the tool surfaces and any calculated numerical noise in the pressure and temperature at the top and bottom contact surfaces. This makes the problem well behaved for the LS-OPT optimization.

Figure 2.




Shvets [6] provides the following function to calculate the heat transfer coefficient.

$$h = h_0\left[1 + 85\left(\frac{P}{\sigma}\right)^{0.8}\right]$$

where P is the applied pressure, $h_0$ is the heat transfer coefficient at P=0, and $\sigma$ is a material hardness metric. $h_0$ and $\sigma$ are parameters to be determined using LS-OPT. The LS-DYNA keywords used to define the pressure dependence of the convection heat transfer coefficient are

```
*PARAMETER
       rho     1000.
    rsigma     1000.
$====== CONVECTION BOUNDARY CONDITIONS =====
$
*BOUNDARY_CONVECTION_SET
$#     sid
         1
$#     fid    lcidh      lcidt      mult
         1        0.        11        1.
$
$================ FUNCTIONS ================
$
*DEFINE_FUNCTION
$#     fid     definition
         1     top surface coefficient
h1=h0*(1.+85.*(20./sigma)**0.8)
```

The LS-DYNA input defines 2 parts (see Fig. 3) because there are 2 parameters ($h_0$ and $\sigma$) to be determined. One part is for P=0 and the other part is for P=20. Table 3 presents the LS-OPT parameters used for the optimization. The results are $h_0$=634.5 and $\sigma$=1193. Figure 4 shows a comparison between the numerical answers and the experimental data for the two cases of P=0 and P=20.

Table 3. LS-OPT input parameters

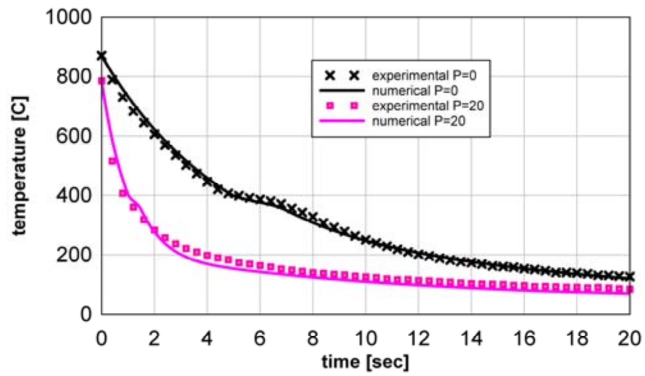
| | |
|---|---|
| Strategy | SRSM – sequential with domain reduction |
| Variables | h0(start, min, max) = 1000, 500, 1500)<br>hard(start, min, max) = (1000, 500, 4000) |
| Sampling | Polynomial, linear, D-Optimal |
| Histories | T_numerical, T_experimental for P=0 @ node point 1<br>T_numerical, T_experimental for P=20 @ node point 5 |
| Response | MeanSqrErr for T_num vs  T_exp for P=0<br>MeanSqrErr for T_num vs  T_exp for P=20 |
| Objective | MeanSqrErr for P=0<br>MeanSqrErr for P=20 |
| Constraints | None |
| Algorithm | LFOP |
| Run | 10 iterations |

**Figure 3. The LS-DYNA model consists of 2 parts, one for P=0 and the other for P=20.**

$$\dot{q} = hA(T_{blank} - T_{\infty})$$

**where** $h = h_0\left[1 + 85\left(\frac{P}{\sigma}\right)^{0.8}\right]$


**Figure 4. Comparison of numerical vs. experimental temperatures using the optimization results $h_0$=634.5, σ=1193.**




### Quenching Heat Transfer Coefficients

This section describes how to use LS-OPT to calculate boiling heat transfer coefficients as a function of temperature for quenching in liquids as shown in Figure 5a. Instead of installing thermocouples on the real part, a small flat plate is used with thermocouples mounted on the top and bottom surfaces. The experimental data [7] consists of temperature-time histories for the 2 thermocouples, Figure 5b. The objective is to use LSOPT to determine the temperature dependent heat transfer coefficients such that the LS-DYNA calculated temperatures match the measured temperatures.

Fig 5a. Water quench

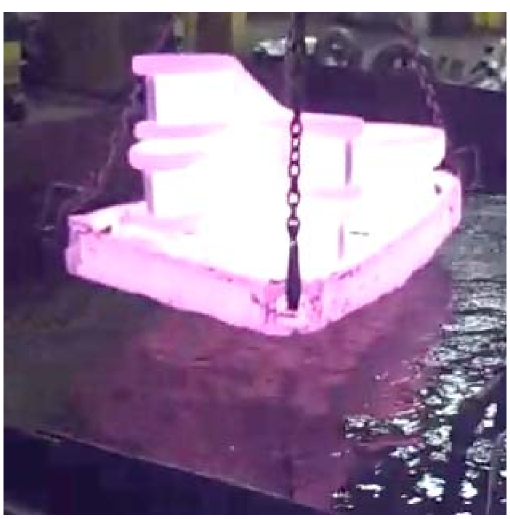
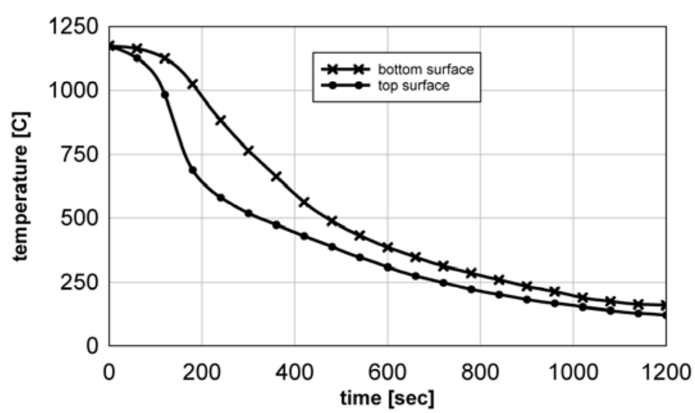


Fig 5b. Measured surface temperatures



Fifteen heat transfer coefficients to be determined where specified as shown in table 5 spanning the temperature range of 75C to 1125C. The LSOPT starting value, lower, and upper bound are also shown in Table 5. The LFOP optimization algorithm was used with a mean squared error objective function between the measured and calculated temperatures on the bottom and top surfaces. Figure 6a shows the calculated temperature history using the optimized heat transfer coefficients in Figure 7a. Note the kink in curve 6a at time=175sec and the noise in the h values in curve 7a at temperature=1100C. Figures 6b and 7b show the results using the GA algorithm. Note that the noise is attenuated. Next, the GA optimized h values were used as the starting point for a 2$^{nd}$ optimization using the LFOP algorithm. The lower and upper bounds where set to ±25% of the starting point values. The results are shown in Figures 6c and 7c. Figure 8 shows a comparison between the measured temperatures and those calculated using the heat transfer coefficients from Figure 7c. The agreement is very good.

Table 5. LSOPT parameters to be determined with their starting point values, lower bound and upper bound. The last column is the optimized answer.

| *DEFINE_CURVE temperature, | parameter | LSOPT parameter value start | lower | upper | Optimized answer (see fig. 7c) h [W/m$^2$C] |
|---|---|---|---|---|---|
| 75. | h1 | 10 | 10 | 500 | 14 |
| 175. | h2 | 100 | 100 | 500 | 236 |
| 275. | h3 | 100 | 100 | 500 | 248 |
| 375. | h4 | 100 | 100 | 500 | 289 |
| 475. | h5 | 100 | 100 | 500 | 319 |
| 575. | h6 | 100 | 100 | 500 | 310 |
| 675. | h7 | 100 | 100 | 500 | 258 |
| 775. | h8 | 100 | 100 | 500 | 242 |
| 825. | h9 | 100 | 100 | 500 | 225 |
| 875. | h10 | 100 | 100 | 500 | 209 |
| 925. | h11 | 100 | 100 | 500 | 193 |
| 975. | h12 | 100 | 100 | 500 | 159 |
| 1025. | h13 | 100 | 100 | 500 | 132 |
| 1075. | h14 | 50 | 50 | 200 | 78 |
| 1125. | h15 | 10 | 10 | 100 | 49 |

Fig 6a. Calculated results using the LFOP algorithm

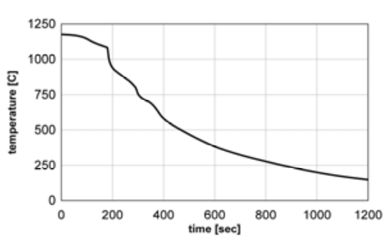



Fig 6b. Calculated results using GA algorithm

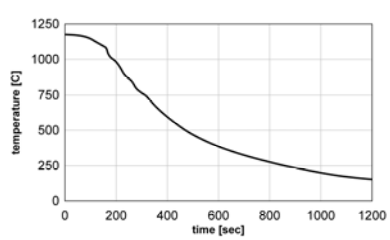



Fig 6c. calculated results after 2$^{nd}$ optimization

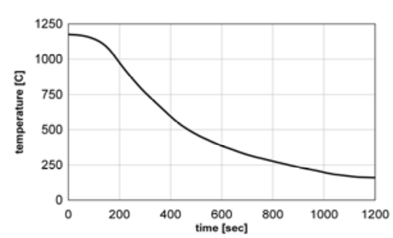


Fig7a. Calculated h values using the LFOP algorithm

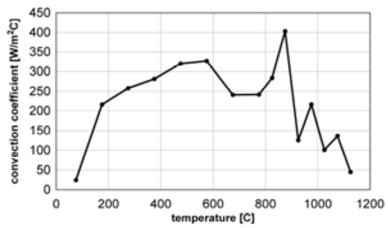



Fig 7b. Calculated h values using the GA algorithm

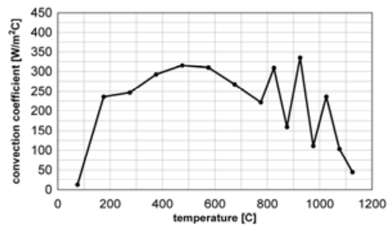



Fig 7c. Calculated h values after the 2nd optimization

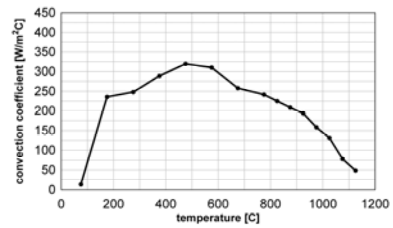
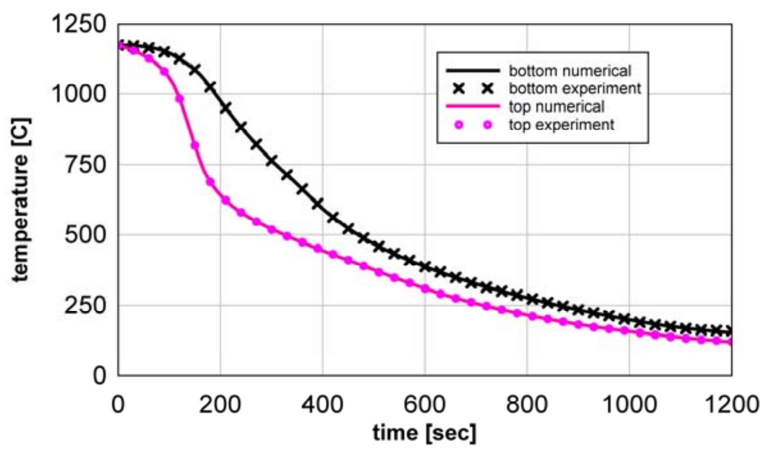



Fig 8. A comparison between the measured temperatures and those calculated using the heat transfer coefficients from Figure 7c.




## References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3. A. Bardelcik, S. Winkler, M.J. Worswick, M.A. Wells, "Investigation of Experimental and Numerical Predictions of Phase Transformations in Hot Stamping at Sub-Critical Cooling Rates", (in Preparation), University of Waterloo, 2011.
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