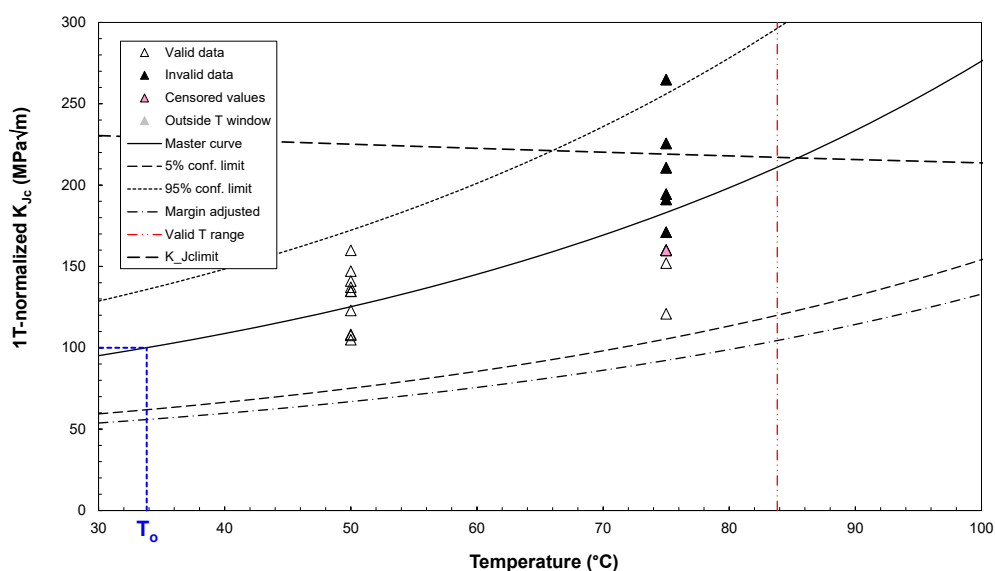


# Spreadsheet-Based Software for the Analysis of Homogeneous and Inhomogeneous Fracture Toughness Data Sets in Accordance with ASTM E1921-21



Enrico Lucon

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NISTIR 8426

# **Spreadsheet-Based Software for the Analysis of Homogeneous and Inhomogeneous Fracture Toughness Data Sets in Accordance with ASTM E1921-21**

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# Abstract

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NIST has developed a user-friendly spreadsheet-based software package for the Master Curve analysis of fracture toughness tests performed in the ductile-to-brittle transition region and the determination of the reference temperature  $T_o$ , in accordance with ASTM E1921-21. The software consists of multiple spreadsheets, which feature several macros that automate most calculations. The software package applies to the analysis of both macroscopically homogeneous and inhomogeneous materials. Complete user's instructions are provided in this report.

The software has been successfully validated using several example problems provided in ASTM E1921-21.

As in the case of previous software packages developed by the Fatigue and Fracture Group of NIST in Boulder, the spreadsheet will be made freely available to the public by contacting the author of this report ([enrico.lucon@nist.gov](mailto:enrico.lucon@nist.gov)).

## Key words

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ASTM E1921-21; ductile-to-brittle transition region; fracture toughness; macroscopically inhomogeneous materials; Master Curve; spreadsheet-based software; reference temperature.

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# 1. Introduction

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ASTM Standard E1921, *Standard Test Method for Determination of Reference Temperature,  $T_o$ , for Ferritic Steels in the Transition Range* [1], covers the determination of a reference temperature,  $T_o$ , which characterizes the fracture toughness of ferritic steels that experience the onset of cleavage cracking corresponding to elastic, or elastic-plastic, instabilities.  $T_o$  corresponds to the temperature at which the median toughness of 1 in. (25.4 mm) thick Compact Tension, C(T), specimens is exactly  $100 \text{ MPa}\sqrt{\text{m}}$ .

E1921 applies to ferritic steels with yield strengths from 275 MPa to 825 MPa and weld metals that have  $\pm 10\%$  or less strength mismatch with respect to the base metal.

The statistical effects of specimen size on the elastic-plastic stress-intensity factor at cleavage,  $K_{Jc}$ , (derived from the  $J$ -integral at fracture,  $J_c$ ) are assessed using the weakest-link theory [2] applied to a three-parameter Weibull distribution of fracture toughness values. A limit on  $K_{Jc}$ ,  $K_{Jc\text{limit}}$ , is set based on specimen size and yield strength, in order to ensure high constraint conditions along the crack front at fracture.

Statistical methods are employed to establish the toughness transition curve as a function of temperature and its specified tolerance bounds for a specific specimen type and thickness of the material tested. The standard deviation of the data distribution is a function of the Weibull slope and the median  $K_{Jc}$ . The toughness transition curve is commonly known as the Master Curve [3], and its placement along the temperature axis is established by means of the reference temperature  $T_o$ .

The statistical methods used in the main body of ASTM E1921-21 assume that the material is macroscopically homogeneous, so that its tensile and toughness properties can be considered relatively uniform. A screening criterion is provided for assessing whether the data set is not representative of a macroscopically homogeneous material, and therefore should not be analyzed using the reference (homogeneous) statistical procedures.

In case the material does not fulfil the homogeneity screening criterion, its fracture toughness can be assessed using alternative analysis methods for macroscopically inhomogeneous materials, detailed in Appendix X5 of the standard.

This report describes the use of three macro-enabled MS Excel<sup>1</sup> spreadsheets, developed at NIST, that can be used to establish the Master Curve and reference temperature of a generic steel, be it macroscopically homogeneous or inhomogeneous. Validation of the spreadsheet-based software is accomplished by comparison with several example problems provided in ASTM E1921-21.

The software package consists of the following MS Excel files:

- *ASTM E1921 - Homogeneous analysis + screening + simplified method.xlsm*: to be used for the analysis of a homogeneous data set, as well as for determining whether the data set can be considered macroscopically inhomogeneous; in such case, a revised Master Curve and reference temperature can be established by means of a simplified method, which can only be used for small data sets.
- *ASTM E1921 - Bimodal analysis.xlsm*: to be used for the analysis of a macroscopically inhomogeneous large data set that contains two distinct toughness populations.

---

<sup>1</sup> Trade names and manufacturers are mentioned in this report only to accurately describe NIST activities. Such inclusion neither constitutes nor implies endorsement by NIST or by the U.S. government.



- *ASTM E1921 - Multimodal analysis.xlsm*: to be used for the analysis of a macroscopically inhomogeneous large data set that contains multiple randomly distributed toughness populations.

This software package is the latest in a series of programs [4-7] for the analysis of various mechanical test data that has been developed at NIST, and can be requested free of charge by contacting the author of this report ([enrico.lucon@nist.gov](mailto:enrico.lucon@nist.gov)).

## 2. Spreadsheet “*ASTM E1921 - Homogeneous analysis + screening + simplified method.xlsm*”

### 2.1. Sheet “*Homogeneous Analysis*”

This sheet performs a complete Master Curve analysis for a macroscopically homogeneous data set in accordance with Section 10 (*Data Analysis and Evaluation of the Reference Temperature,  $T_o$* ) of ASTM E1921-21.

#### 2.1.1. Data input and preliminary calculations

The top portion of the sheet (Figure 1), starting with row {15}, is used to input basic information about the data set to be analyzed<sup>2</sup>:

- Cell {C9}: name/basic info on the data set analyzed.
- Column {A}: codes/ID for the specimen tested.
- Column {B}: test temperatures ( $^{\circ}\text{C}$ ).
- Column {C}: initial crack sizes,  $a_o$  (mm).
- Column {D}: specimen widths,  $W$  (mm).
- Column {E}: specimen thicknesses,  $B$  (mm).
- Column {G}: ductile crack extensions preceding cleavage,  $\Delta a$  (mm).
- Column {H}: values of stress intensity factor at the onset of cleavage,  $K_{Jc}$  ( $\text{MPa}\sqrt{\text{m}}$ ).
- Column {N}: notes/comments on individual tests/specimens.

The remaining columns in the table contain data that are automatically calculated for each test, and should not be changed by the user:

- Column {F}: specimen ligament sizes,  $b_o = W - a_o$  (mm).
- Column {I}: yield strength at test temperature,  $\sigma_{ys}$  (MPa).
- Column {J}: elastic/Young’s modulus at test temperature,  $E$  (GPa).
- Column {K}: maximum specimen  $K_{Jc}$  capacity, given by  $K_{Jclimit} = \sqrt{\frac{Eb_o\sigma_{ys}}{30(1-\nu^2)}}$ , where  $\nu$  is Poisson’s ratio.
- Column {L}: whether the data point is censored (YES/NO), due to either  $K_{Jc} > K_{Jclimit}$  or excessive crack growth, or both.<sup>3</sup> Censored values are highlighted in **dark red** over pink background.

<sup>2</sup> Here, and in all other spreadsheets, cells that require direct input from the user are identified by a **yellow background**.

<sup>3</sup> If the test exhibited excessive crack growth or if  $K_{Jc} > K_{Jclimit}$ , the respective  $\Delta a$  or  $K_{Jc}$  values in columns {G} or {H} are highlighted in **bold red**.

- Column {M}:  $K_{Jc}$  values to be used in subsequent analyses, *i.e.*,  $K_{Jc}$  from column {H} for an uncensored data point,  $K_{Jc,limit}$  if  $K_{Jc} > K_{Jc,limit}$ , or  $K_{Jc\Delta a}^4$  in case of excessive crack growth.

The maximum number of data points (tests) that can be analyzed is 340. Empty/unused row in the table can be hidden by clicking [HIDE UNUSED ROWS]. Rows can be unhidden by clicking the button [UNHIDE ROWS]. All existing data in the table can be erased by clicking the button [CLEAR DATA].

**Determination of Reference Temperature,  $T_0$ , for Ferritic Steels in the Transition Range**  
ASTM E1921-21

Analysis for Homogeneous Materials - Multi-Temperature Approach

**1. Material characteristics**

Fit coefficients

	$\sigma_{YS}$ (MPa)	$E$ (GPa)	$\sigma_{YS,RT}$ (MPa)
[2 <sup>nd</sup> order term] A =	0.00E+00	0	646
[1 <sup>st</sup> order term] B =	-0.5349	-0.0625	
(Intercept) C =	661.16	204	

If yield strength is to be calculated from a polynomial fit (cells L8:L10), leave this cell blank.

**2. Dimensional and crack growth requirements**

(Excessive crack growth) (Above  $K_{Jc,lim}$ )

Specimen code/ID	T (°C)	$\sigma_u$ (mm)	W (mm)	B (mm)	$b_p$ (mm)	$\Delta a$ (mm)	$K_{Jc}$ (MPa√m)	$\sigma_{YS}$ (MPa)	E (GPa)	$K_{Jc,lim}$ (MPa√m)	Censored? (YES/NO)	$K_{Jc,analyzed}$ (MPa√m)	Test Notes
MW11D	90	27.25	50.80	25.40	23.55	0.000	112.60	610.14	198.38	323.10	NO	112.60	
MW11A	90	25.43	50.80	25.40	25.37	0.152	162.70	610.14	198.38	335.41	NO	162.70	
MW91D	90	27.23	50.80	25.40	23.57	0.000	151.60	610.14	198.38	323.27	NO	151.60	
MW91A	90	25.93	50.80	25.40	24.87	2.108	208.90	610.14	198.38	332.04	YES	240.00	
MW9MN	90	25.91	50.80	25.40	24.89	2.667	259.50	610.14	198.38	332.21	YES	240.00	
MW91C	90	25.45	50.80	25.40	25.35	7.620	325.10	610.14	198.38	335.24	YES	240.00	
MW91B	90	26.72	50.80	25.40	24.08	4.318	307.00	610.14	198.38	326.74	YES	240.00	
MW9KD	75	26.80	50.80	25.40	24.00	0.000	110.30	616.74	199.31	328.75	NO	110.30	
MW11JD	75	26.85	50.80	25.40	23.95	0.000	115.20	616.74	199.31	328.41	NO	115.20	
MW11KD	75	26.54	50.80	25.40	24.26	0.000	134.90	616.74	199.31	330.49	NO	134.90	
MW9NA	75	26.75	50.80	25.40	24.05	0.559	183.60	616.74	199.31	329.10	NO	183.60	
MW11LB	75	26.87	50.80	25.40	23.93	0.737	211.90	616.74	199.31	328.23	NO	211.90	
MW91C	75	26.67	50.80	25.40	24.13	0.635	240.00	616.74	199.31	329.62	NO	240.00	
MW11JC	75	27.74	50.80	25.40	23.06	7.925	345.10	616.74	199.31	322.25	YES	240.00	
MW91B	75	27.00	50.80	25.40	23.80	2.032	260.70	616.74	199.31	327.36	YES	240.00	
MW11LFB	50	12.86	25.20	12.60	12.34	0.000	107.10	629.12	200.88	239.05	NO	107.10	
MW11MCA	50	12.73	25.20	12.60	12.47	0.000	132.80	629.12	200.88	240.27	NO	132.80	
MW9LEB	50	12.88	25.20	12.60	12.32	0.000	133.80	629.12	200.88	238.80	NO	133.80	
MW11HEB	50	13.24	25.20	12.60	11.96	0.000	176.10	629.12	200.88	235.33	NO	176.10	
MW9HEA	50	12.80	25.20	12.60	12.40	1.499	217.30	629.12	200.88	239.54	YES	240.00	

**3. Application of the multi-temperature approach for the calculation of the reference temperature**

USE TEMPERATURE LIMITS? [YES] T limits (°C) -28.2 71.8

Specimen T  $K_{Jc(0.001)}$   $K_{Jc,LT}$   $\delta_1$   $r_1$   $n_1$  Equation (20)

Homogeneous Analysis Homogeneity Screening Procedure Simplified Method Result Summary

Figure 1 - Upper portion of sheet "Homogeneous Analysis" (sections 1 and 2).

Information about the material's tensile properties can be input in cell block {L8-N12}. For both the material's yield strength,  $\sigma_{YS}$ , and Young's modulus,  $E$ , the user can input fitting coefficients assuming polynomial regressions of the form  $Y = AT^2 + BT + C$ , where  $T$  is test temperature. Note that ASTM E1921-21 provides the following equation for estimating  $E$  as a function of test temperature  $T$ :

$$E = 204 - \frac{T}{16}, \quad (1)$$

with  $E$  in GPa and  $T$  in °C.

If only the yield strength at room temperature,  $\sigma_{YS,RT}$ , is known, E1921-21 recommends the use of the following equation [8]:

$$\sigma_{YS} = \sigma_{YS,RT} + \frac{10^5}{491 + 1.8T} - 189, \quad (2)$$

with  $\sigma_{YS}$  in MPa and  $T$  in °C.

<sup>4</sup> According to Section 10.2.1 of E1921-21,  $K_{Jc\Delta a}$  corresponds to the highest uncensored  $K_{Jc}$  value in the data set.

If a value for  $\sigma_{YS,RT}$  is entered in cell {N8}, it is used to calculate yield strength values in column {I} according to eq. (2)<sup>5</sup>. If cell {N8} is left blank, a polynomial fit based on the fitting coefficients in cells {L8-L10} is used.

The value of Poisson's ratio,  $\nu$ , is entered in cell {M12}.

Two navigation buttons are available in the upper part of the sheet, column {O}:

- **[CALCULATIONS]**: selects cell {A356}, at the beginning of the Calculation section.
- **[MC PLOT]**: selects cell {A1066}, corresponding to the top of the Master Curve plot.

### 2.1.2. Calculation of the Reference Temperature, $T_o$

The reference temperature,  $T_o$ , is calculated by means of the multi-temperature approach. This is the reference method in ASTM E1921-21, and consists of iteratively solving the following equation:

$$\sum_{i=1}^N \delta_i \frac{\exp[0.019 (T_i - T_{oQ})]}{11 + 77 \exp[0.019 (T_i - T_{oQ})]} - \sum_{i=1}^N \frac{(K_{Jc(i)} - 20)^4 \exp[0.019 (T_i - T_{oQ})]}{\{11 + 77 \exp[0.019 (T_i - T_{oQ})]\}^5} = 0 \quad (3)$$

where  $T_i$  and  $K_{Jc(i)}$  are the test temperature and the result (uncensored or censored) of the  $i^{\text{th}}$  test in the data set, respectively, and  $T_{oQ}$  is a provisional value of the reference temperature.  $\delta_i$  is 1 for an uncensored datum and 0 if the datum is censored.

Although E1921 provides a direct evaluation method for calculating  $T_{oQ}$  in case all tests are conducted at the same temperature (*single temperature analysis*), the spreadsheet handles single-temperature data sets in the same way as multi-temperature data sets, *i.e.*, iteratively solving eq. (3) above.

The middle portion of the sheet (Figure 2) is used for the calculation of  $T_{oQ}$  and its validation as  $T_o$ .

356

A

B

C

D

E

F

G

H

I

J

K

L

M

N

357

3. Application of the multi-temperature approach for the calculation of the reference temperature

T limits (°C)

358

Specimen

T

K<sub>Jc,anal</sub>

K<sub>Jc,LT</sub>

δ<sub>i</sub>

r<sub>i</sub>

n<sub>i</sub>

Equation (20)

359

code

(°C)

(MPa√m)

(MPa√m)

1<sup>st</sup> member

2<sup>nd</sup> member

360

MW11LD

90

112.6

112.6

0

0

0.000

0.0000

0.0000

361

MW11JA

90

162.7

162.7

0

0

0.000

0.0000

0.0000

362

MW91D

90

151.6

151.6

0

0

0.000

0.0000

0.0000

363

MW9LA

90

240.0

240.0

0

0

0.000

0.0000

0.0000

364

MW9MN

90

240.0

240.0

0

0

0.000

0.0000

0.0000

365

MW91C

90

240.0

240.0

0

0

0.000

0.0000

0.0000

366

MW9JB

90

240.0

240.0

0

0

0.000

0.0000

0.0000

367

MW9KD

75

110.3

110.3

0

0

0.000

0.0000

0.0000

368

MW11JD

75

115.2

115.2

0

0

0.000

0.0000

0.0000

369

MW11KD

75

134.9

134.9

0

0

0.000

0.0000

0.0000

370

MW9NA

75

183.6

183.6

0

0

0.000

0.0000

0.0000

371

MW11LB

75

211.9

211.9

0

0

0.000

0.0000

0.0000

372

MW9JC

75

240.0

240.0

0

0

0.000

0.0000

0.0000

373

MW11JC

75

240.0

240.0

0

0

0.000

0.0000

0.0000

374

MW9LB

75

240.0

240.0

0

0

0.000

0.0000

0.0000

375

MW11LFB

50

107.1

93.1

1

1

0.167

0.0120

0.0008

376

MW11MCA

50

132.8

114.7

1

1

0.167

0.0120

0.0023

377

MW9LEB

50

133.8

115.5

1

1

0.167

0.0120

0.0024

378

MW11HEB

50

176.1

151.0

1

1

0.167

0.0120

0.0086

379

MW9HEA

50

240.0

204.6

0

0

0.000

0.0000

0.0338

380

381

699

700

USE TEMPERATURE LIMITS?

YES

NO

(T<sub>o</sub> - 50 °C ≤ T ≤ T<sub>o</sub> + 50 °C)

Sum of 1<sup>st</sup> member:

0.048

Sum of 2<sup>nd</sup> member:

0.048

Difference:

0.000

SOLVE

T<sub>oQ</sub> =

21.8

°C

(not valid per ASTM E1921)

Σ<sub>i</sub>

r<sub>i</sub>n<sub>i</sub>

=

0.7

# tests =

20

N =

5

r =

4

K<sub>min</sub> =

20

MPa√m

K<sub>Jc,Δσ</sub> =

240.0

MPa√m

K<sub>o,eq</sub> =

162.0

MPa√m

K<sub>med,eq</sub> =

149.5

MPa√m

Figure 2 - Middle portion of sheet "Homogeneous Analysis" (section 3): example of an invalid reference temperature.

<sup>5</sup> In this case, cells {L8-L10} are **grayed out**.

Only data points corresponding to temperatures in the range  $T_{oQ} \pm 50$  °C should be used for the calculation of the reference temperature. These limits are shown in cells {N357,N358}. However, in some cases when the iterative solution of eq. (3) does not converge, it may be advantageous to perform a preliminary  $T_{oQ}$  calculation using all tests in the data set, regardless of their temperature. A drop-down menu is available to the user in cell {M357} for applying or ignoring temperature limits. After calculating  $T_{oQ}$  without using the limits, these should be reinstated before performing the final evaluation.

The results of the iterative calculations are displayed in cells {M360} (first member of eq. (3)), {M362} (second member), and {M364} (difference between the two members). Calculations are launched by clicking [SOLVE]<sup>6</sup>. Cell {M364} turns **green** if the two members are equal or **red** if the difference is  $\neq 0$ .

The validity of  $T_{oQ}$  depends on whether

$$\sum_{i=1}^3 r_i n_i \geq 1 \quad , \quad (4)$$

where:  $r_i$  is the number of uncensored data within the  $i^{\text{th}}$  temperature range ( $50$  °C  $\leq T_i \leq -14$  °C,  $-15$  °C  $\leq T_i \leq -35$  °C, or  $-36$  °C  $\leq T_i \leq -50$  °C), and  $n_i$  is the corresponding weighting factor (1/6, 1/7, or 1/8, respectively). If the requirement above, eq. (4), is fulfilled, then  $T_{oQ} = T_o$ . Information on the validity/invalidity of  $T_{oQ}$  is displayed in cells {K368-M368}.

Additional parameters calculated and displayed in this section are:

- Number of tests performed, cell {L372}
- Number of data points within the  $T_{oQ} \pm 50$  °C limits (if used),  $N$ , cell {L373}
- Number of uncensored data,  $r$ , cell {L374}
- Lower bound of toughness used in the Weibull analysis ( $K_{min} = 20$  MPa $\sqrt{\text{m}}$ ), cell {L376}
- Crack extension censoring limit,  $K_{Jc\Delta a}$ , corresponding to the highest uncensored  $K_{Jc}$  value in the data set, cell {L377}
- Scale parameter of the Weibull model for a multi-temperature data set,  $K_{o,eq}$ , cell {L379}
- Median toughness of a multi-temperature data set,  $K_{med,eq}$ , cell {L381}.

### 2.1.3. Plot of Master Curve and tolerance bounds

In the lower part of the sheet, the obtained Master Curve is plotted, along with experimental data points and tolerance bounds. The user sets up the plot by entering the initial temperature and the temperature interval (step) for plotting the Master Curve and its tolerance bounds (Figure 3) in cells {A1048} and {A1050}, both highlighted in **yellow**.

Values of  $T_i$ ,  $K_{Jc(i)}$ , and  $K_{Jc,IT}$  (toughness values converted to  $IT$  equivalence) are listed starting in cells {B707}, {C707}, and {D707}, respectively. Data points for the  $IT$ -equivalent Master Curve, its 5 % and 95 % confidence bounds, and the 5 % margin-adjusted lower bound<sup>7</sup>, are displayed starting in cells {E1047-H1047}.

This section of the sheet (Figure 3) also displays the margin adjustment corresponding to an 85 % confidence level, cell {C703}, and the estimated standard deviation of  $T_o$ , cell {G703}, which for both sample size and experimental uncertainties.

<sup>6</sup> The reference temperature is obtained through the use of the SOLVER tool of MS Excel. The solving method used is GRG Nonlinear, with the following options: constraint precision = 0.000001, integer optimality = 5 %, max time = 100 s, iteration limit = 100, convergence = 0.001.

<sup>7</sup> The margin adjustment, described in Section 10.9 of ASTM E1921-21, is an upward temperature shift of the 5 % tolerance bound, which covers the uncertainty in  $T_o$  caused by the use of a limited number of test specimens.

701	4. Master curve fit to data																	
702																		
703	Margin adj. (85 % conf.):	14.2	°C (est.)		Stand. dev. on $T_o$ =	9.8	°C (est.)											
704																		
705		T	$K_{Jc,1T}$	$K_{Jc,1T}$	$K_{Jc,1T}$	5% conf.	95% conf.	5% L.B.										
706		(°C)	(MPa√m)	(MPa√m)	(MPa√m)	(MPa√m)	(MPa√m)	(MPa√m)										
707		90	112.6	112.6														
708		90	162.7	162.7														
709		90	151.6	151.6														
710		90	208.9	208.9														
711		90	259.5	259.5														
712		90	325.1	325.1														
713		90	307.0	307.0														
714		75	110.3	110.3														
715		75	115.2	115.2														
716		75	134.9	134.9														
717		75	183.6	183.6														
718		75	211.9	211.9														
719		75	240.0	240.0														
720		75	345.1	345.1														
721		75	260.7	260.7														
722		50	107.1	93.1														
723		50	132.8	114.7														
724		50	133.8	115.5														
725		50	176.1	151.0														
726		50	217.3	185.6														
1047	Start T (°C)	20			97.6	60.6	132.3	52.3										
1048	20				111.7	68.0	152.8	57.9										
1049	Step T (°C)	40			128.8	77.0	177.5	64.8										
1050	10				149.5	87.8	207.5	73.0										
1051	Min test T (°C)	60			174.5	100.9	243.7	83.0										
1052	50				204.8	116.7	287.4	95.1										
1053	Max test T (°C)	80			241.4	135.9	340.4	109.7										
1054	90				285.6	159.0	404.4	127.4										
1055	Max $K_{Jc,1T}$	100			339.1	187.0	481.8	148.8										
1056	345.1	110			403.7	220.9	575.3	174.7										
1057		120			482.0	261.8	688.5	205.9										
1058		130			576.5	311.3	825.4	243.8										
1059		140			690.9	371.2	990.9	289.5										
1060		150			829.2	443.6	1191.0	344.8										

Figure 3 - Lower portion of sheet "Homogeneous Analysis" (section 4): experimental data points and Master Curve with associated tolerance bounds.

The chart at the very bottom of the sheet (Figure 4) displays the following:

- valid (uncensored) data;
- invalid (censored) data;
- replacement data for invalid data;
- data falling outside the temperature limits;
- Master Curve for 1T specimens;
- 5 % and 95 % tolerance bounds;
- margin-adjusted 5 % lower bound;
- temperature limits (if included in the scale of the X-axis);
- maximum  $K_{Jc}$  capacity,  $K_{Jc,limit}$ , as a function of temperature (only if selected from the drop-down menu in cell {N1068})<sup>8</sup>.

The user must select the scale of the X (abscissa) and Y (ordinate) axis (using the information on minimum and maximum test temperature, and maximum value of  $K_{Jc,1T}$  provided in cells {A1052}, {A1054}, and {A1056}, respectively), as well as manually position the label corresponding to  $T_o$ .

The second line of the chart title corresponds to the “Material specifications” info that the user has input in cell {C9}.

<sup>8</sup> The  $K_{Jc,limit}$  curve is calculated using the average value of ligament size,  $W-a_o$ , for the specimens tested. If specimens of different size have been tested, the  $K_{Jc,limit}$  curve does not make sense, and should not be plotted.

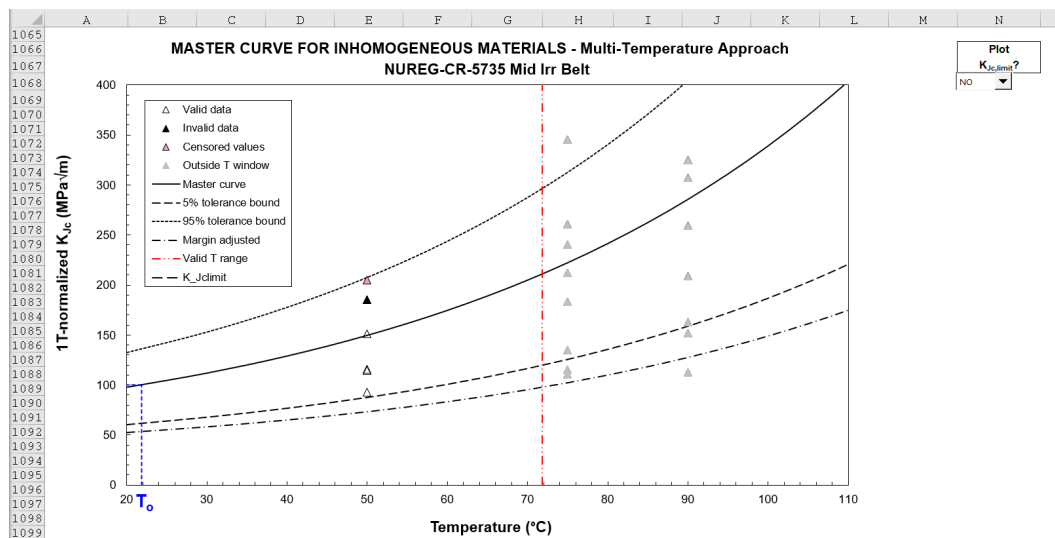


Figure 4 – Master Curve chart (section 4).

## 2.2. Sheet “Homogeneity Screening Procedure”

The homogeneity screening procedure described in section 10.6 of ASTM E1921-21, based on the SINTAP<sup>9</sup> method [9], is implemented in this sheet.

### 2.2.1. Data censoring

Section 1 of the sheet (Figure 5) performs censoring of the data set. Every 1T-equivalent censored datum ( $\delta_i = 0$  in column {F}) is replaced in the analysis by  $K_{CENS}$ , which corresponds to the median (Master Curve) toughness value at the same test temperature, calculated for the benchmark  $T_o$  value displayed in cell {K11}. At the beginning of the analysis, the benchmark value corresponds to the reference temperature from the homogeneous analysis, and is copied from the sheet “E1921-21 Multi-T” by clicking [COPY FROM HOMOGENEOUS ANALYSIS]. For uncensored data,  $K_{analysis} = K_{Jc, 1T}$ .

<sup>9</sup> SINTAP (Structural Integrity Assessment Procedures for European Industry) was a European Union Brite-Euram Program that was conducted in the second half of the 1990s.

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Determination of Reference Temperature,  $T_0$ , for Ferritic Steels in the Transition Range

ASTM E1921-20

GO TO...

CALCULATIONS

Homogeneity Screening Procedure based on SINTAP method

1. Data censoring

UNHIDE ROWS

HIDE UNUSED ROWS

Specimen code	T (°C)	$K_{JCE0.5}$ (MPa $\sqrt{m}$ )	$K_{JCE1T}$ (MPa $\sqrt{m}$ )	$K_{CE0.5}$ (MPa $\sqrt{m}$ )	$\delta_1$	$K_{analysis}$ (MPa $\sqrt{m}$ )
MW11LD	90	112.6	112.6	231.3	1	112.6
MW11JA	90	162.7	162.7	231.3	1	162.7
MW91D	90	151.6	151.6	231.3	1	151.6
MW9LA	90	208.9	208.9	231.3	1	208.9
MW9MN	90	259.5	259.5	231.3	0	231.3
MW91C	90	325.1	325.1	231.3	0	231.3
MW91B	90	307.0	307.0	231.3	0	231.3
MW9KD	75	110.3	110.3	181.4	1	110.3
MW11JD	75	115.2	115.2	181.4	1	115.2
MW11KD	75	134.9	134.9	181.4	1	134.9
MW9NA	75	183.6	183.6	181.4	0	181.4
MW11LB	75	211.9	211.9	181.4	0	181.4
MW91C	75	240.0	240.0	181.4	0	181.4
MW11JC	75	345.1	345.1	181.4	0	181.4
MW91B	75	260.7	260.7	181.4	0	181.4
MW11LFB	50	107.1	93.1	124.1	1	93.1
MW11MCA	50	132.8	114.7	124.1	1	114.7
MW91EB	50	133.8	115.5	124.1	1	115.5
MW11HEB	50	176.1	151.0	124.1	0	124.1
MW9HEA	50	217.3	185.6	124.1	0	124.1

Benchmark  $T_0$  = 34.4 °C

COPY FROM HOMOGENEOUS ANALYSIS

Figure 5 – Data censoring in the Homogeneity Screening Procedure (section 1).

In this part of the sheet, buttons for hiding/unhiding rows and jumping to the CALCULATIONS section are provided (Figure 5).

### 2.2.2. New estimate of $T_o$

The second part of the sheet (Figure 6) recalculates  $T_o$  based on the censored data set obtained in the first part. Once again, temperature limits ( $\pm 50$  °C) can be used or ignored<sup>10</sup>, and  $T_o$  is calculated by clicking **[Find T0]**.

The value of  $T_o$  in cell {I363} is compared with the value calculated in the previous step ( $T_o$  from the homogeneous analysis for the first iteration). If the difference  $T_{o(step\ n)} - T_{o(step\ n-1)}$  does not exceed 0.5 °C, the analysis must continue, and the user must click **[Copy value as benchmark  $T_o$ ]** to determine a new censored data set in section 1. If the difference is less than 0.5 °C, the analysis is completed, and the corresponding message is displayed in cells {H365-J365}.

The following 2-step cycle must be repeated until the “**NO – Analysis Completed**” message appears:

- Click **[Find T0]**.
- Click **[Copy value as benchmark  $T_o$ ]**.

<sup>10</sup> Once again, if convergence is not achieved (difference value in cell {J360}  $\neq 0$ ), the following procedure is recommended: (a) exclude temperature limits by selecting “NO” in the drop-down menu in cell {L353}; (b) calculate  $T_o$ ; (c) enable temperature limits by selecting “YES” in the drop-down menu; (d) recalculate  $T_o$ .



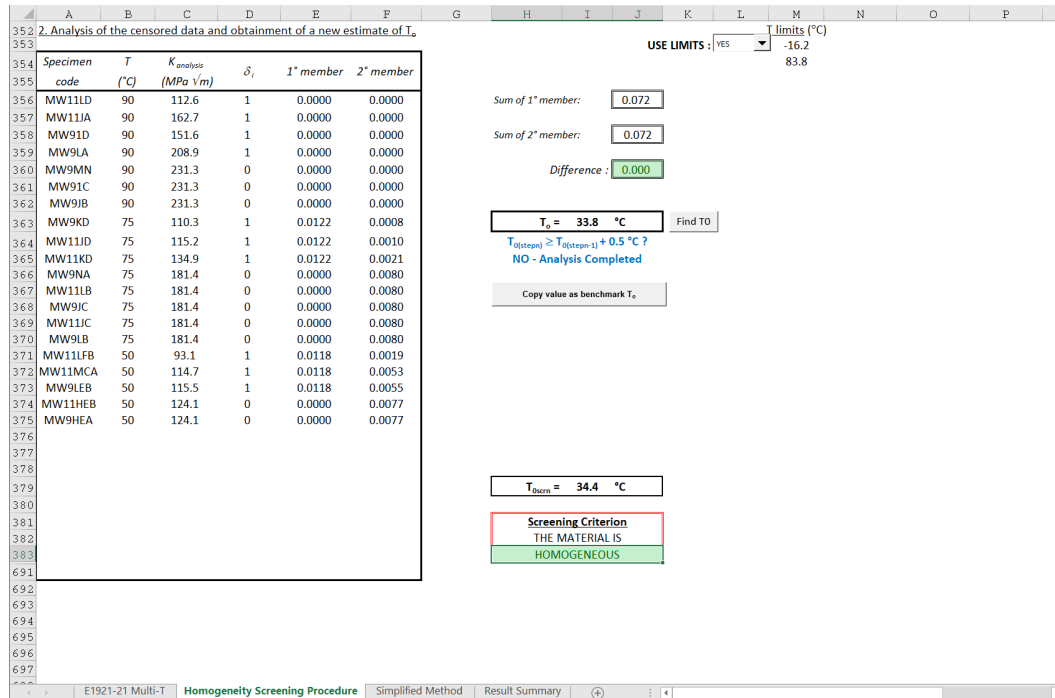


Figure 6 – Analysis section of the Homogeneity Screening Procedure (section 2).

Once the analyses are completed, the maximum value of the individual  $T_{o(step\ i)}$ , which is defined as  $T_{oscrn}$ , is shown in cell {I379}. If:

$$T_{oscrn} - T_{o(step1)} \leq 1.44 \sqrt{\frac{\beta^2}{r}} \quad , \quad (5)$$

with  $\beta$  = sample size uncertainty factor corresponding to  $T_{o(step1)}$  (determined in accordance with Section 10.9.1 of E1921-21), the data set is considered to be representative of a material that is macroscopically homogeneous. If the inequality in eq. (5) is not satisfied, the data set can be considered representative of a macroscopically inhomogeneous material.

Cells {H383-J383} display the color-coded outcome of the screening procedure: **HOMOGENEOUS** or **INHOMOGENEOUS**.

### 2.3. Sheet “Simplified Method”

A simplified method [10] for treating macroscopically inhomogeneous data sets is implemented in this sheet. This method must be used for small data sets ( $N < 20$ ).

If  $N \leq 9$ , every uncensored data point is associated to a single-data estimate given by:

$$T_{oi} = T_i - \frac{\ln \left[ \frac{(K_{JC(i)} - 20) N^{0.25-10}}{70} \right]}{0.019} \quad . \quad (6)$$

The highest value of  $T_{oi}$  is defined as  $T_{omax}$ . If this latter value is higher than  $T_{oscrn}$  (as previously determined) by more than 8 °C, then  $T_{oIN} = T_{omax}$ . Otherwise,  $T_{oIN} = T_{oscrn}$ . If  $10 \leq N < 20$ ,  $T_{oIN} = T_{oscrn}$  always.



$T_{oIN}$  is a generally conservative estimate of the material's reference temperature, and should be used in place of  $T_o$ . This sheet is structurally similar to the sheet “E1921-21 Multi-T”, see Figure 7 (section 1), Figure 8 (section 2), and Figure 9 (Master Curve plot). The value calculated for  $T_{oIN}$  is shown in cell {J17}.

Determination of Reference Temperature, $T_o$ , for Ferritic Steels in the Transition Range ASTM E1921-21															
Determination of the Reference Temperature for Inhomogeneous Materials (Simplified Method)															
1. Calculation of the maximum value of $T_o$ (based on a single data point) and establishment of $T_o$ for the data set															
Specimen id	T (°C)	$K_{Jd(exp)}$ (MPa√m)	$K_{Jd}$ (MPa√m)	$\delta_5$	$T_{oI}$ (°C)										
MW11LD	90	112.6	112.6	0											
MW11IA	90	162.7	162.7	0											
MW91D	90	151.6	151.6	0											
MW9LA	90	208.9	240.0	0											
MW9MN	90	259.5	240.0	0											
MW91C	90	325.1	240.0	0											
MW9JB	90	307.0	240.0	0											
MW9KD	75	110.3	110.3	0											
MW11JD	75	115.2	115.2	0											
MW11KD	75	134.9	134.9	0											
MW9NA	75	183.6	183.6	0											
MW11LB	75	211.9	211.9	0											
MW91C	75	240.0	240.0	0											
MW11IC	75	345.1	240.0	0											
MW9LB	75	260.7	240.0	0											
MW11LFB	50	107.1	93.1	1	31.6										
MW11MCA	50	132.8	114.7	1	16.8										
MW9LEB	50	133.8	115.5	1	16.3										
MW11HEB	50	176.1	151.0	1	-1.4										
MW9HEA	50	217.3	204.6	0											

$T_{o,max} = 31.6 \text{ } ^\circ\text{C}$

$T_{o,scrn} = 34.4 \text{ } ^\circ\text{C}$

$T_{o,max} - T_{o,scrn} > 8 \text{ } ^\circ\text{C}$ : **NO**  
 Number of tests  $N = 5$   
 $T_{oIN} = 34.4 \text{ } ^\circ\text{C}$

Figure 7 – Sheet “Simplified Method”: section 1.

2. Final Master Curve fit to data							
Margin adj. (85 % conf.):		14.2	$^\circ\text{C}$ (est.)		Stand. dev. on $T_o = 9.8 \text{ } ^\circ\text{C}$ (est.)		
T (°C)	$K_{Jd(exp)}$ (MPa√m)	$K_{Jd(1T)}$ (MPa√m)	$K_{MC(1T)}$ (MPa√m)	5% conf. (MPa√m)	95% conf. (MPa√m)	5% L.B. (MPa√m)	
90.0	112.6	112.6					
90.0	162.7	162.7					
90.0	151.6	151.6					
90.0	240.0	240.0					
90.0	240.0	240.0					
90.0	240.0	240.0					
90.0	240.0	240.0					
75.0	110.3	110.3					
75.0	115.2	115.2					
75.0	134.9	134.9					
75.0	183.6	183.6					
75.0	211.9	211.9					
75.0	240.0	240.0					
75.0	240.0	240.0					
75.0	240.0	240.0					
50.0	107.1	93.1					
50.0	132.8	114.7					
50.0	133.8	115.5					
50.0	176.1	151.0					
50.0	240.0	204.6					
Start T (°C)	20		83.2	53.4	111.8	46.8	
20	30		94.4	59.3	128.0	51.2	
Step T (°C)	40		107.9	66.4	147.6	56.7	
10	50		124.1	75.0	171.2	63.2	
Min test T (°C)	60		143.9	85.4	199.8	71.2	
50	70		167.7	98.0	234.4	80.8	
Max test T (°C)	80		196.5	113.2	276.3	92.4	
90	90		231.3	131.6	326.8	106.5	
Max $K_{Jd}$ (MPa√m)	100		273.4	153.8	388.0	123.5	
345.1	110		324.4	180.7	462.0	144.0	
	120		386.0	213.2	551.4	168.8	
	130		460.5	252.6	659.6	198.9	
	140		550.6	300.1	790.4	235.2	
	150		659.5	357.6	948.5	279.1	
	160		791.2	427.2	1139.8	332.3	

Figure 8 – Sheet “Simplified Method”: section 2 (upper portion).

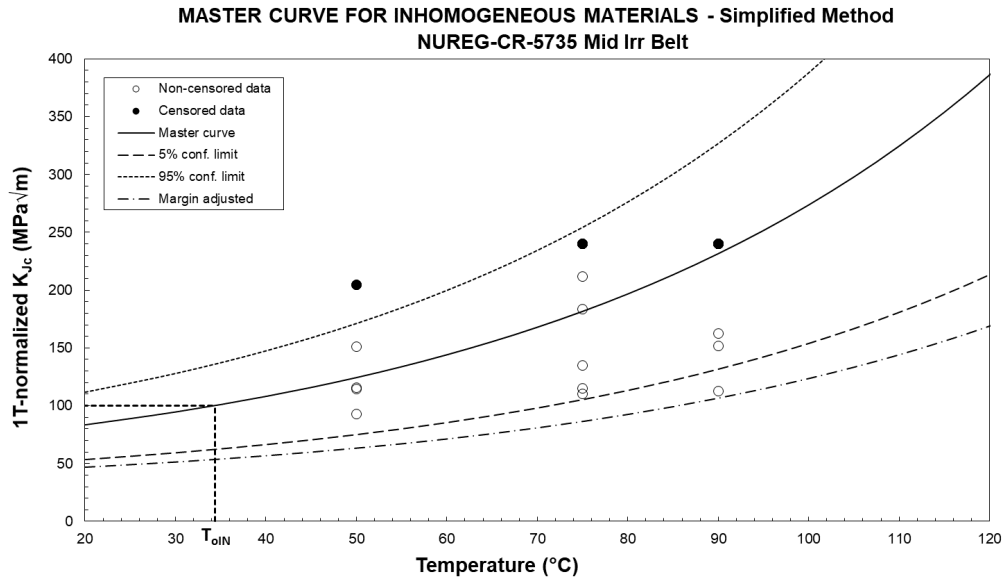


Figure 9 – Sheet “*Simplified Method*”: Master Curve plot.

This sheet should not be used if:

- the data set is screened to be macroscopically homogeneous in the sheet “*Homogeneity Screening Procedure*”, or
- $N \geq 20$  (in this case, the spreadsheets “*ASTM E1921 - Bimodal analysis.xlsm*” or “*ASTM E1921 - Multimodal analysis.xlsm*” should be used).

## 2.4. Sheet “*Result Summary*”

The results of the analyses performed are summarized in this sheet (Figure 10), and can be printed on the default system printer by clicking [PRINT RESULTS]. The cells highlighted in yellow must be filled in by the user, who must also select the specimen type from the drop-down menu in cells {C6-E6} and the location of displacement measurement from the drop-down menu in cell {F13}. The validity of  $T_o$  shall be indicated in cell {H20}, along with the reason(s) for invalidity, if applicable, in cells {D21-H21}.

The specific results reported are:  $r$ ,  $N$ ,  $K_{Jc\Delta a}$ ,  $K_o$ ,  $K_{Jc(med)}$ ,  $T_{oQ}$  or  $T_o$ ,  $T_{oscrn}$ , and whether the material is classified as homogeneous or inhomogeneous.

### NOTES:

- if “Other” has been selected for either the specimen type or the location of displacement measurement, comments/clarifications must be entered in cells {B29-G32}.
- If the material is classified as inhomogeneous, the values of  $T_{omax}$  and  $T_{oIN}$  are displayed in cells {H25} and {H26}, respectively.

	A	B	C	D	E	F	G	H	I	J	K
1	<b>MASTER CURVE ANALYSES FOR THE</b>										<b>PRINT RESULTS</b>
2	<b>DETERMINATION OF THE REFERENCE TEMPERATURE, <math>T_0</math></b>										
3	<b>ASTM E1921-21</b>										
4											
5	<b>Material analyzed:</b>		NUREG-CR-5735 Mid Irr Belt								
6	<b>Specimen type:</b>		Compact Tension, C(T)								
7	<b>Nominal thickness <math>B</math>:</b>		12.6-25.4 mm								
8	<b>Nominal net thickness <math>B_N</math>:</b>		mm								
9	<b>Nominal width <math>W</math>:</b>		25.2-50.8 mm								
10											
11	<b>Number of uncensored data, <math>r</math>:</b>			4		<b>Number of specimens tested, <math>N</math>:</b>			5		
12											
13	<b>Location of displacement measurement:</b>			Load-line							
14											
15	<b>Ductile crack growth limit:</b>		$K_{IC, \Delta \sigma} \approx$		240.0		MPa $\sqrt{m}$				
16	<b>Weibull scale parameter:</b>		$K_{\sigma} \approx$		162.0		MPa $\sqrt{m}$				
17	<b>Median fracture toughness:</b>		$K_{IC(med)} \approx$		149.5		MPa $\sqrt{m}$				
18											
19											
20	<b>Master Curve reference temperature:</b>			$ToQ \approx$		21.8		°C		<b>Valid:</b> NO	
21	<b>Reason for invalidity:</b>			Sum $r_i/n_i < 1$							
22											
23	<b>Screening reference temperature:</b>			$T_{0scm} \approx$		34.4		°C			
24											
25	<b>Material is classified as:</b>			HOMOGENEOUS							
26											
27											
28	<b>COMMENTS</b>										
29											
30											
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40											

E1921-21 Multi-T
Homogeneity Screening Procedure
Simplified Method
Result Summary

Figure 10 – Sheet “Result Summary”

### 3. Analysis of potentially inhomogeneous large ( $N \geq 20$ ) data sets

If the data set under investigation has been screened as macroscopically inhomogeneous using the homogeneous analysis (Section 2) and includes at least 20 tests ( $N \geq 20$ ), two additional methods to assess material inhomogeneity are provided in Annex X5 of ASTM E1921-21 (*Treatment of Potentially Inhomogeneous Data Sets*). These methods [11] allow a more accurate determination of the likelihood that the material is inhomogeneous with respect to the screening criterion described in Section 2.2, and a more reliable characterization of material performance within the ductile-to-brittle transition regime than the simplified method of Section 2.3.

One of these methods (Section 3.1) applies to data sets that exhibit a bimodal toughness distribution, while the other method (Section 3.2) can be used for a data set that is characterized by a multimodal distribution. It’s important to note that, when a data set is found to be potentially inhomogeneous, it is not possible to analytically determine the nature of the inhomogeneity (that is, if the data set corresponds to a bimodal or multimodal

material). Information on the origin of the specimen data set, fabrication and location of the test specimens, and processing of the material may suggest which inhomogeneity model is most likely to apply. If a physical basis to determine the nature of the inhomogeneity is unavailable, both the bimodal and the multimodal analyses should be performed, and the result that leads to the most conservative assessment should be selected.

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### 3.1. Worksheet “*Bimodal analysis.xlsm*”

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The bimodal toughness distribution applies to data sets that contain two toughness populations, one more brittle than the other. Examples of such materials are heat-affected zone (HAZ) materials, where the crack tip can sample either the base or the weld material.

#### 3.1.1. Sheet “*Bimodal Analysis*”

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Input data must be entered by the user in cell {C1} (information on the data set/material analyzed) and columns {A-E}, starting in row {11} (specimen/test id, test temperature,  $K_{Jc}$ ,  $K_{JcIT}$ , and  $\delta_i$ , respectively). Data in columns {A-D} should be just copied from the homogeneous analysis, while  $\delta_i$  values should be carefully checked by the user in every step of the analysis:  $\delta_i = 0$  if  $K_{Jc} > K_{Jc\text{limit}}$  or if  $T$  lies outside  $(T_B - 50\text{ }^\circ\text{C})$  or  $(T_A + 50\text{ }^\circ\text{C})$ , where  $T_A$  and  $T_B$  are the reference temperatures of the two toughness populations.<sup>11</sup>

Previous data can be erased by clicking [CLEAR DATA]. A maximum of 1000 data points can be analyzed in this spreadsheet.

Other data that must be entered by the user before performing the analysis are:

- Cell {B3}: initial value of the probability of sampling a specimen from population A<sup>12</sup>,  $p_A$ ; should be set to 0.5.
- Cell {B4}: initial value of  $T_A$ ; should be set 20 °C above the reference temperature from the homogeneous analysis,  $T_A = T_o + 20\text{ }^\circ\text{C}$ .
- Cell {B5}: initial value of  $T_B$ ; should be set 20 °C below the reference temperature from the homogeneous analysis,  $T_B = T_o - 20\text{ }^\circ\text{C}$ .

The analysis is launched by clicking [SOLVE], which maximizes the logarithm of the likelihood in cell {F7} through the use of the SOLVER algorithm of MS Excel. The results are displayed in cells {B3-B5} ( $p_A$ ,  $T_A$ ,  $T_B$ ), as well as cell {D3} ( $p_B = 1 - p_A$ ).

The upper left portion of this sheet is shown in Figure 11.

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<sup>11</sup>  $\delta_i$  values are highlighted in dark red on pink background if the test temperature falls outside the valid  $T$  range.

<sup>12</sup> By convention, A is the population with the lower toughness (more brittle component).

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Data set analyzed: ASTM E1921-20 Section X5.5.2							CLEAR DATA								
2																
3	$p_A = 0.56$		$p_B = 0.44$		$N = 53$				$\sigma_{T_A} = 4.18$		$^{\circ}\text{C}$		$MLNH = 3.52$		$T_A - T_B = 24.5$	
4	$T_A = -33.6$		$^{\circ}\text{C}$		$r = 49$				$\sigma_{T_B} = 3.85$		$^{\circ}\text{C}$		$MLNH_{ec} = 3.44$		$MLNH \text{ confidence } \approx 85 \%$	
5	$T_B = -58.1$		$^{\circ}\text{C}$		$K_{min} = 20$		$\text{MPa}\sqrt{\text{m}}$		$\sigma_{p_A} = 0.066$				==> DATASET LIKELY NON HOMOGENEOUS			
6	Valid temperature range															
7	X Outside valid T range				$\ln L = -243.5$		SOLVE		$T_B - 50\text{ }^{\circ}\text{C} = -108$		$^{\circ}\text{C}$		$T_A + 50\text{ }^{\circ}\text{C} = 16$		$^{\circ}\text{C}$	
8																
9	Specimen	T	$K_{Ic}$	$K_{IcIT}$	$\delta_I$	$K_{Q,A}$	$K_{Q,B}$	Fraction A	Fraction B	Expon A	Expon B	$f_i$	$S_i$	$(\ln L_i)$		
10	id	( $^{\circ}\text{C}$ )	( $\text{MPa}\sqrt{\text{m}}$ )	( $\text{MPa}\sqrt{\text{m}}$ )		( $\text{MPa}\sqrt{\text{m}}$ )	( $\text{MPa}\sqrt{\text{m}}$ )									
11	Sample 1	-80	51.3	46.3	1	62.9	81.8	0.005387706	0.001252	0.141805	0.032953	0.0126182	0.911605	-4.37262		
12	Sample 2	-80	87.9	77.1	1	62.9	81.8	0.055002214	0.012781469	3.140454	0.729782	0.0161589	0.235895	-4.12528		
13	Sample 3	-80	113.4	98.5	1	62.9	81.8	0.143156635	0.033266879	11.24348	2.612772	0.0042884	0.032203	-5.45184		
14	Sample 4	-65	73.9	73.9	1	73.4	98.5	0.019247211	0.004119736	1.037425	0.222054	0.0210984	0.550403	-3.85856		
15	Sample 5	-65	126.8	126.8	1	73.4	98.5	0.149732221	0.032049171	15.9914	3.422851	0.001836	0.014321	-6.30017		
16	Sample 6	-55	167.7	144.2	1	82.3	112.6	0.026003967	0.006963202	15.81516	3.229703	0.0018071	0.017373	-6.31604		
17	Sample 7	-55	88.5	77.6	1	82.3	112.6	0.012702253	0.002593999	0.731668	0.149418	0.0176355	0.647989	-4.03784		
18	Sample 8	-55	115.2	100.1	1	82.3	112.6	0.034097293	0.006963202	2.729602	0.557428	0.0119949	0.288033	-4.42327		
19	Sample 9	-55	81.4	71.6	1	82.3	112.6	0.009147747	0.001868113	0.472308	0.096453	0.0157782	0.748467	-4.14912		
20	Sample 10	-55	121.9	105.7	1	82.3	112.6	0.041814952	0.008539269	3.583012	0.731707	0.0098222	0.22681	-4.62311		
21	Sample 11	-55	145.0	125.1	1	82.3	112.6	0.077186099	0.015762611	8.113189	1.65684	0.005332	0.083912	-5.23403		
22	Sample 12	-55	104.2	90.8	1	82.3	112.6	0.023590944	0.004817641	1.670321	0.341106	0.0159768	0.417719	-4.13662		
23	Sample 13	-55	64.4	57.3	1	82.3	112.6	0.003459059	0.000706394	0.129147	0.026374	0.0080294	0.92061	-4.82464		
24	Sample 14	-55	96.8	84.6	1	82.3	112.6	0.017901636	0.003655795	1.156103	0.236094	0.0177114	0.523256	-4.03355		
25	Sample 15	-55	114.5	99.5	1	82.3	112.6	0.033350663	0.006810728	2.650201	0.541213	0.0122477	0.295168	-4.40242		
26	Sample 16	-55	107.4	93.5	1	82.3	112.6	0.026384165	0.00538806	1.939087	0.395992	0.0148835	0.376169	-4.2075		
27	Sample 17	-55	81.0	71.3	1	82.3	112.6	0.008970126	0.00183184	0.46012	0.093964	0.015633	0.753749	-4.15837		
28	Sample 18	-55	70.0	62.0	1	82.3	112.6	0.004939991	0.001008807	0.207698	0.042415	0.0107035	0.876562	-4.53718		
29	Sample 19	-55	131.8	114.0	1	82.3	112.6	0.05522484	0.011277778	5.19181	1.060249	0.0075494	0.155192	-4.88629		
30	Sample 20	-55	69.5	61.6	1	82.3	112.6	0.00479319	0.000978845	0.199514	0.040744	0.0104602	0.881011	-4.56018		
31	Sample 21	-55	67.5	59.9	1	82.3	112.6	0.004235356	0.000864926	0.169171	0.034547	0.0094917	0.897787	-4.65734		
32	Sample 22	-30	102.3	89.2	1	113.5	162.3	0.004344275	0.000808595	0.300649	0.055959	0.0085594	0.830447	-4.76073		
33	Sample 23	-30	194.0	166.3	1	113.5	162.3	0.041054954	0.007641512	6.006996	1.118075	0.0046138	0.144909	-5.3787		
34	Sample 24	-30	170.4	146.5	1	113.5	162.3	0.02651315	0.004934862	3.35314	0.624116	0.0067236	0.254832	-5.00213		
35	Sample 25	-30	129.5	112.1	1	113.5	162.3	0.010231992	0.001904469	0.942143	0.17536	0.0117557	0.587083	-4.44341		
36	Sample 26	-30	118.2	102.6	1	113.5	162.3	0.007379931	0.001373618	0.609405	0.113428	0.0111565	0.696943	-4.49574		
37	Sample 27	-30	147.9	127.6	1	113.5	162.3	0.016305325	0.003034892	1.753648	0.326405	0.0101801	0.413902	-4.58732		
38	Sample 28	-30	178.8	153.5	1	113.5	162.3	0.031208243	0.005808755	4.167372	0.775668	0.0057815	0.210826	-5.15309		
39	Sample 29	-30	95.9	83.8	1	113.5	162.3	0.003407557	0.000634245	0.217484	0.04048	0.0072211	0.872939	-4.93075		
40	Sample 30	-20	135.1	135.1	1	130.7	189.8	0.010148404	0.001835954	1.168081	0.211318	0.0096911	0.529851	-4.63655		
41	Sample 31	-20	108.9	108.9	1	130.7	189.8	0.004676028	0.000845943	0.415699	0.075204	0.0083015	0.777401	-4.79131		
42	Sample 32	-20	177.1	177.1	1	130.7	189.8	0.025804791	0.00466836	4.053933	0.733399	0.0049423	0.220597	-5.30992		
43	Sample 33	-20	141.7	141.7	1	130.7	189.8	0.011996195	0.002170239	1.459937	0.264118	0.0091782	0.467418	-4.69092		
44	Sample 34	-20	174.4	174.4	1	130.7	189.8	0.024497044	0.004431774	3.787344	0.684266	0.0051778	0.234254	-5.26338		
45	Bimodal Analysis Confidence MLNH (bimodal) Master Curve chart Result Summary															

Figure 11 – Upper left portion of the sheet “Bimodal Analysis”.

The likelihood that the data set is inhomogeneous is assessed by calculating the parameter  $MLNH^{13}$ , which is shown in cell {L3}, while cell {L4} displays the exceedance criterion  $MLNH_{ec}$ , which is established by linear interpolation of the values provided in Table X5.1 of ASTM E1921-21 as a function of  $N^{14}$ . If  $MNLH > MLNH_{ec}$ , the data set is defined as “likely not homogeneous”; if  $MNLH \leq MLNH_{ec}$ , the analysis is “unable to guarantee material inhomogeneity”. The outcome of the inhomogeneity check is displayed in cells {L5-O5}. If  $N < 20$ , the message becomes “Data set cannot be analyzed ( $N < 20$ )”. Finally, if  $MNLH$  cannot be calculated and is therefore labeled as “UNDEFINED”, the message displayed is “The data set cannot be analyzed using this method”.

The percent confidence,  $MNLH_{conf}$ , in the  $MLNH$  evaluation for correctly identifying a material as inhomogeneous is a function of  $N$ ,  $T_A - T_B$ , and  $p_A$ , as shown by Monte Carlo analyses in [12], and is evaluated in the separate sheet “Confidence MLNH (multimodal)”. Specifically, if  $T_A - T_B \leq 30$  °C,  $p_A \geq 0.8$ , or  $p_A \leq 0.2$ , the confidence in the  $MNLH$  evaluation is poor.  $MNLH_{conf}$  can be calculated by linearly interpolating the values reported in Table X5.2 of ASTM E1921-21.

The bimodal Master Curve and corresponding tolerance bounds cannot be calculated analytically, but are obtained by satisfying the following relationship:

<sup>13</sup>  $MLNH$  is an acronym for Maximum Likelihood of Non-Homogeneity.

<sup>14</sup> In Table X5.1 of ASTM E1921-21, values of  $MLNH_{ec}$  are provided for  $N = 20, 32$ , and  $64$ . If  $N > 64$ ,  $MLNH_{ec}$  is estimated using  $N = 64$ , as the results will be conservative.

$$S = 1 - 0.xx, \quad (7)$$

where the selective cumulative failure probability,  $S$ , is given by:

$$S = p_A \exp \left[ - \left( \frac{K_{JC(0.xx)} - 20}{K_A(T_i) - 20} \right)^4 \right] + (1 - p_A) \exp \left[ - \left( \frac{K_{JC(0.xx)} - 20}{K_B(T_i) - 20} \right)^4 \right], \quad (8)$$

and  $xx$  is the selected cumulative failure probability.

The establishment of the 98 % and 2 % tolerance bounds<sup>15</sup> is performed in the right side of the “*Bimodal Analysis*” sheet (Figure 12). The user must input the initial temperature value in cell {S5} and the temperature step in cell {V5}, then click [FIT MC 98 %] for the first tolerance bound and [FIT MC 2 %] for the second tolerance bound. If convergence is not achieved by clicking these buttons (for example, because the values displayed in column {R} are too different than the actual target values), then the user must click the individual [FIT] buttons in column {Y}. Acceptable convergence is achieved when the sums of residuals in cells {X33,X48} is of the order of  $10^{-6}$ .

P	Q	R	S	T	U	V	W	X	Y
	Min test T =		-80 °C			Max test T =	0 °C		
	Initial T value:		-90 °C		Step:	12 °C			
	T	Master Curves							
	(°C)	$K_{0,A}$	$K_{0,B}$						
	-90	57.2	72.8						
	-78	64.0	83.5						
	-66	72.4	97.0						
	-54	83.0	113.9						
	-42	96.4	135.1						
	-30	113.1	161.8						
	-18	134.2	195.3						
	-6	160.6	237.3						
	6	193.8	290.2						
	18	235.5	356.6						
	T	Master Curve (failure probability = 98 %)							
	(°C)	$K_{0,98\%}$	$K_{0,A}$	ExponA	$K_{0,B}$	ExponB	S	Residual	FIT MC 98 %
	-90	90.0	57.2	12.48385	72.8	3.088937	0.02	8.44E-07	FIT
	-78	104.2	64.0	13.45018	83.5	3.088936	0.02	4.42E-07	FIT
	-66	122.0	72.4	14.35865	97.0	3.088892	0.02	4.9E-08	FIT
	-54	144.4	83.0	15.19188	113.9	3.088892	0.02	2.36E-07	FIT
	-42	172.6	96.4	15.93868	135.1	3.088849	0.02	5.56E-07	FIT
	-30	207.9	113.1	16.59536	161.8	3.088875	0.02	7.71E-09	FIT
	-18	252.4	134.2	17.16261	195.3	3.088888	0.02	2.67E-07	FIT
	-6	308.1	160.6	17.64561	237.3	3.08891	0.02	7.14E-07	FIT
	6	378.2	193.8	18.05131	290.2	3.088851	0.02	4.54E-07	FIT
	18	466.2	235.5	18.38955	356.6	3.088901	0.02	5.41E-07	FIT
							Sum	4.11E-06	
	T	Master Curve (failure probability = 2%)							
	(°C)	$K_{0,2\%}$	$K_{0,A}$	ExponA	$K_{0,B}$	ExponB	S	Residual	FIT MC 2 %
	-90	35.5	57.2	0.030266	72.8	0.007489	0.98	6.73E-07	FIT
	-78	38.4	64.0	0.03063	83.5	0.007034	0.98	9.67E-07	FIT
	-66	42.0	72.4	0.030936	97.0	0.006555	0.98	2.07E-07	FIT
	-54	46.5	83.0	0.031187	113.9	0.006341	0.98	4.6E-07	FIT
	-42	52.1	96.4	0.031394	135.1	0.006084	0.98	1.81E-07	FIT
	-30	59.2	113.1	0.031561	161.8	0.005874	0.98	5.04E-07	FIT
	-18	68.2	134.2	0.0317	195.3	0.005705	0.98	9.22E-07	FIT
	-6	79.4	160.6	0.031809	237.3	0.005568	0.98	6.63E-07	FIT
	6	93.4	193.8	0.031897	290.2	0.005458	0.98	5.52E-08	FIT

Figure 12 – Upper right portion of the sheet “*Bimodal Analysis*”.

### 3.1.2. Sheet “*Confidence MLNH (bimodal)*”

As indicated above, the confidence associated with the accuracy of *MNLH* to correctly identify a material as inhomogeneous is evaluated in this sheet, through the calculation of the *MNLH<sub>conf</sub>* parameter. Note that if  $N > 64$  or  $T_A - T_B > 50$  °C (maximum values in Table X5.2 of E1921-21), calculations assume  $N = 64$  and  $T_A - T_B = 50$  °C, as the results will be conservative.

<sup>15</sup> If other levels of failure probability are desired for the tolerance bounds (for example, 95 % and 5 %), it will be sufficient to replace “0.02” and “0.98” with “0.05” and “0.95” in cells {X9-X18} and {X23-X32}, respectively.

The user should not modify this sheet, which doesn't require any external input.

### 3.1.3. Sheet “*Master Curve chart*”

The bimodal Master Curves for population A and population B, and the associated 98 % and 2 % tolerance bounds are plotted in this sheet, along with the experimental data points (Figure 13). The scales of the X and Y axis are automatically determined, but can be modified by the user.

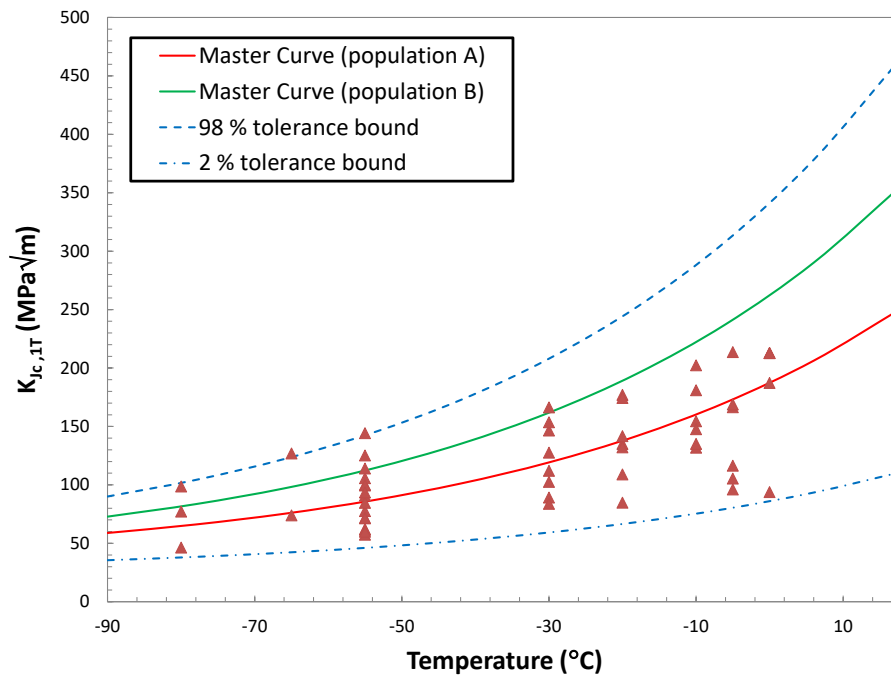


Figure 13 – Bimodal Master Curve chart.

### 3.1.4. Sheet “*Result Summary*”

The results of the bimodal analyses performed are summarized in this sheet (Figure 14), and can be printed on the default system printer by clicking **[PRINT RESULTS]**. The cells highlighted in yellow must be filled in by the user, who must also select the specimen type from the drop-down menu in cells {C6-E6} and the location of displacement measurement from the drop-down menu in cell {F13}.

The specific results reported are:  $MLNH$ ,  $MNLH_{ec}$ ,  $MLNH_{conf}$ ,  $p_A$ ,  $p_B$ ,  $T_A$ ,  $T_B$ , and whether the material is classified as homogeneous or inhomogeneous.

**NOTE:** if “Other (see Comments)” has been selected for either the specimen type or the location of displacement measurement, comments/clarifications must be entered in cells {B21-G25}.



	A	B	C	D	E	F	G	H	I	J	K
1	<b>ASTM E1921-21</b>										PRINT RESULTS
2	<b>TREATMENT OF POTENTIALLY INHOMOGENEOUS DATA SETS</b>										
3	<b>Bimodal Method</b>										
4											
5	Material/data set analyzed: ASTM E1921-20 Section X5.5.2										
6	Specimen type: Compact Tension, C(T)										
7	Nominal thickness B: 25 mm										
8	Nominal net thickness B <sub>N</sub> : 20 mm										
9	Nominal width W: 50 mm										
10											
11	Location of displacement measurement: Other (see Comments)										
12											
13	MLNH = 3.52 MLNH <sub>ref</sub> = 3.44 MLNH <sub>corr</sub> = 85 %										
14											
15	p <sub>A</sub> = 0.56										
16	T <sub>A</sub> = -33.6 °C										
17	T <sub>B</sub> = -58.1 °C										
18	Material is determined to be: INHOMOGENEOUS										
19											
20											
21	COMMENTS										
22											
23											
24											
25											
26											
	Bimodal Analysis Confidence MLNH (bimodal) Master Curve chart Result Summary										

Figure 14 – Sheet “Result Summary”.

## 3.2. Worksheet “Multimodal analysis.xlsm”

The multimodal toughness distribution applies to data sets that contain randomly distributed toughness populations. Examples of such materials are heterogeneous ferritic steels, for which macroscopic heterogeneities are randomly distributed, or data sets of similar materials that have been combined together. Individually, each separate population follows the Master Curve distribution. Two parameters fully define the combined (multimodal) distribution: the mean reference temperature of all populations,  $T_m$ , and its standard deviation around the mean,  $\sigma_{Tm}$ .

### 3.2.1. Sheet “Multimodal Analysis”

Input data is be entered by the user in cell {C1} (information on the data set/material analyzed) and columns {I-M}, starting in row {3} (specimen/test id, test temperature,  $K_{Jc}$ ,  $K_{JcIT}$ , and  $\delta_i$ , respectively). Data in columns {I-M} should be just copied from the homogeneous analysis, while  $\delta_i$  values should be carefully checked by the user in every step of the analysis:  $\delta_i = 0$  if  $K_{Jc} > K_{Jc\text{limit}}$  or if  $T$  lies outside  $(T_m - 50 \text{ °C})$  or  $(T_m + 50 \text{ °C})$ , where  $T_m$  is the multimodal reference temperature.<sup>16</sup>

Previous data can be erased by clicking [CLEAR DATA]. A maximum of 120 data points can be analyzed in this spreadsheet.

Additional data that must be entered by the user before performing the analysis are:

- Cell {B3}: initial value of  $T_m$ ; should be set to the reference temperature from the homogeneous analysis ( $T_o$  or  $T_{oQ}$ ).
- Cell {B4}: initial value of  $\sigma_{Tm}$ ; should be set to the value of  $\sigma_{T_o}$  (standard deviation of the reference temperature in the homogeneous analysis).

<sup>16</sup>  $\delta_i$  values are highlighted in dark red on pink background if the test temperature falls outside the valid  $T$  range.





where  $xx$  is the selected cumulative failure probability, and the selective cumulative failure probability,  $S$ , is given by:

$$S = \int_{-\infty}^{\infty} \frac{1}{\sigma_{T_m} \sqrt{2\pi}} \exp \left[ \frac{-(\tau_0 - T_m)^2}{2\sigma_{T_m}^2} \right] \exp \left[ - \left( \frac{K_{Jc(0.xx)} - 20}{K_{\tau_0}(T) - 20} \right)^4 \right] d\tau_0 \quad (8)$$

with  $\tau_0$  = temperature region for calculating the cumulative failure and survival densities, and  $K_{\tau_0}(T)$  = Weibull scale parameter for a population characterized by a reference temperature  $\tau_0$  at the test temperature  $T$ , given by:

$$K_{\tau_0}(T) = 31 + 77 \exp[T_i - \tau_0] \quad . \quad (9)$$

Practically, the infinite integral in eq. (9) can be solved with sufficient accuracy over the range -200 °C to 200 °C.

The determination of the 98 % and 2 % tolerance bounds<sup>17</sup> is performed in the right side of the “*Multimodal Analysis*” sheet (Figure 16), by executing the following steps:

- (a) Input the initial temperature for the calculations in cell {T1}. To help with this selection and the next, minimum and maximum test temperature are shown in cells {T13} and {T14}, respectively.
- (b) Input the temperature step for the calculations in cell {W1}.
- (c) Input the initial  $T$  value in cell {W5}. The corresponding value in cell {R5} is highlighted in **dark red** with pink background.
- (d) Click [**SOLVE**] in cells {W13} ( $K_{Jc,98\%}$ ) and {W21} ( $K_{Jc,2\%}$ ). Convergence<sup>18</sup> is achieved when the values in cells {W12} ( $S_{2\%}$ ) and {W20} ( $S_{98\%}$ ) become 0.02 and 0.98, respectively – both in **green** with light green background.
- (e) Click [**COPY**] to paste the calculated  $K_{Jc,xx\%}$  values in cells {T5} and {U5}. The next temperature value (cell {R6}) automatically becomes highlighted.
- (f) Repeat step (d) and click [**COPY**] in cell {W6}, and so on, until all temperatures are accounted for.

The multimodal Master Curve values ( $K_{Jc,50\%}$ ) are calculated analytically, and are displayed in cell {S5-S11}.

<sup>17</sup> If other levels of failure probability are desired for the tolerance bounds (for example, 95 % and 5 %), the user must replace “0.02” with “0.05” in the macro “Solve\_98”, and “0.98” with “0.95” in the macro “Solve\_2”.

<sup>18</sup> If convergence is not achieved immediately, it is suggested to manually adjust the values in cell {W9} and/or {W20} on the basis of the expected numbers, and click [**SOLVE**] again until calculations converge.

	Q	R	S	T	U	V	W	X
1		Initial T value: -90 °C				Step: 20		
2								
3		T	MC 50 %	MC 98 %	MC 2 %		T	
4		(°C)	(MPa√m)	(MPa√m)	(MPa√m)		(°C)	
5		-90	59.13	91.56	35.25	COPY	30	
6		-70	72.59	118.24	40.23	COPY		
7		-50	92.28	157.30	47.47	COPY	$K_{IC,98\%}$	
8		-30	121.07	214.44	58.04	COPY	(MPa√m)	
9		-10	163.17	298.03	73.48	COPY	599.04	
10		10	224.73	420.27	96.04	COPY	$S_{2\%}$	
11		30	314.75	599.04	129.01	COPY	0.02	
12							SOLVE	
13		Min test T = -80 °C					$K_{IC,2\%}$	
14		Max test T = 0 °C					(MPa√m)	
15							129.01	
16							$S_{98\%}$	
17							0.98	
18							SOLVE	
19								
20		Start by inputting initial T value from cell T1, then click both "SOLVE" buttons and then "COPY" on the left. Proceed in the same way for the remaining T values in the table.						
21								
22								
23								
24								
25								
26								

Figure 16 – Upper right portion of the sheet “Multimodal Analysis”.

### 3.2.2. Sheet “Confidence MLNH (multimodal)”

As indicated above, the confidence associated with the accuracy of *MNLH* to correctly identify a material as inhomogeneous is evaluated in this sheet, through the calculation of the  $MNLH_{conf}$  parameter. Note that if  $N > 64$  (maximum value in Table X5.3 of E1921-21), calculations assume  $N = 64$ , as the results will be conservative.

The user should not modify this sheet, which doesn’t require any external input.

### 3.2.3. Sheet “Master Curve chart”

The multimodal Master Curve and its associated 98 % and 2 % tolerance bounds are plotted in this sheet, along with the experimental data points (Figure 17). The scales of the X and Y axis are automatically determined, but can be modified by the user.

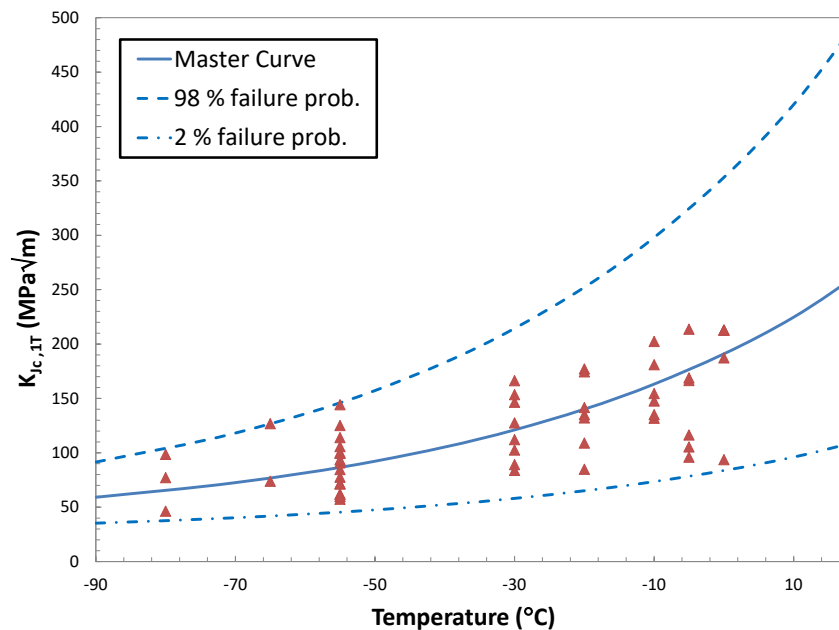


Figure 17 – Multimodal Master Curve chart.

### 3.2.4. Sheet “*Result Summary*”

The results of the multimodal analyses performed are summarized in this sheet (Figure 18), and can be printed on the default system printer by clicking [PRINT RESULTS]. The cells highlighted in yellow must be filled in by the user, who must also select the specimen type from the drop-down menu in cells {C6-E6} and the location of displacement measurement from the drop-down menu in cell {F11}.

The specific results reported are:  $MLNH$ ,  $MNLH_{ec}$ ,  $MLNH_{conf}$ ,  $T_m$ ,  $\sigma_{Tm}$ , and whether the material is classified as homogeneous or inhomogeneous.

NOTE: if “Other (see Comments)” has been selected for either the specimen type or the location of displacement measurement, or both, comments/clarifications must be entered in cells {B20-G24}.

	A	B	C	D	E	F	G	H	I	J	K	L
1	<b>ASTM E1921-21</b>											
2	<b>TREATMENT OF POTENTIALLY INHOMOGENEOUS DATA SETS</b>											
3	<b>Multimodal Method</b>											
4												
5	Material/data set analyzed: <b>ASTM E1921-21 Section X5.5.2</b>											
6	Specimen type: Other (see Comments) ▼											
7	Nominal thickness B: various mm											
8	Nominal net thickness B <sub>N</sub> : various mm											
9	Nominal width W: various mm											
10												
11	Location of displacement measurement: Other (see Comments) ▼											
12												
13	MLNH = 2.77    MLNH <sub>ec</sub> = 2.00    MLNH <sub>conf</sub> = 74%											
14												
15	T <sub>m</sub> = -43.8 °C											
16	σ <sub>Tm</sub> = 13.2 °C											
17												
18	Material is determined to be: <b>INHOMOGENEOUS</b>											
19												
20	COMMENTS											
21												
22												
23												
24												
25												
26												
27												

Figure 18 – Sheet “*Result Summary*”

## 4. Software Validation: ASTM E1921-21 Examples (Appendix X1, X2, X3, X5)

### 4.1. Homogeneous Analyses

#### 4.1.1. Appendix X1, Section X1.2

Section X1.2 of ASTM E1921-21 present the results of the Master Curve analysis of a data set consisting of six C(T) specimens with thickness  $B = 4$  in. = 101.6 mm of A533B steel (nuclear reactor pressure vessel steel), all tested at  $-75$  °C. None of the  $K_{Jc}$  data require censoring.

Table 1 compares the analysis results reported in Section X1.2 of E1921-21 and those obtained from the NIST spreadsheet “*ASTM E1921 - Homogeneous analysis + screening + simplified method.xlsm*”.

Table 1 - Comparison between ASTM E1921-21 Section X1.2 and NIST software results.

Parameter Analysis	$N$	$r$	$K_o$ (MPa√m)	$K_{Jc(med)}$ (MPa√m)	$T_o$ (°C)
ASTM E1921-21	6	6	123.4	114.1	-84.7
NIST software	6	6	123.0	114.0	-84.6
Difference ASTM/NIST	0	0	0.4	0.1	-0.1

#### 4.1.2. Appendix X1, Sections X1.3.1-X1.3.5

Sections X1.3.1 to X1.3.5 of ASTM E1921-21 describe an artificially generated data set consisting of six 1/2TC(T) and six 1TC(T) specimens, all tested at  $38$  °C. Three of the 1/2TC(T)  $K_{Jc}$  data need censoring due to violation of  $K_{Jc limit}$ .

Table 2 compares the results of the analyses reported in E1921-21 and obtained from the NIST spreadsheet “*ASTM E1921 - Homogeneous analysis + screening + simplified method.xlsm*”.

Table 2 - Comparison between ASTM E1921-21 Sections X1.3.1-X1.3.5 and NIST software results.

Parameter Analysis	$N$	$r$	$K_o$ (MPa√m)	$K_{Jc(med)}$ (MPa√m)	$T_o$ (°C)
ASTM E1921-21	12	9	190.0	174.7	-0.2
NIST software	12	9	189.4	174.6	-0.2
Difference ASTM/NIST	0	0	0.6	0.1	0.0

#### 4.1.3. Appendix X1, Sections X1.3.6-X1.3.7

Sections X1.3.6 and X1.3.7 of ASTM E1921-21 describe a similar artificially generated data set consisting of six 1/2TC(T) and six 1TC(T) specimens, all tested at  $38$  °C, but this time it is assumed that the steel has a low upper shelf, so that 10 of the 12 specimens exhibited stable crack growth preceding cleavage. Censoring is therefore due to violation of either or both  $K_{Jc limit}$  and  $K_{JC\Delta a}$ .

Table 3 compares the results of the analyses reported in E1921-21 and obtained from the NIST spreadsheet “*ASTM E1921 - Homogeneous analysis + screening + simplified method.xlsm*”.

Table 3 - Comparison between ASTM E1921-21 Sections X1.3.6-X1.3.7 and NIST software results.

Parameter Analysis	$N$	$r$	$K_{Jc\Delta a}$ (MPa√m)	$K_o$ (MPa√m)	$K_{Jc(med)}$ (MPa√m)	$T_o$ (°C)
ASTM E1921-21	12	7	195.2	189.0	173.8	0.1
NIST software	12	7	195.2	188.4	173.6	0.2
Difference ASTM/NIST	0	0	0	0.6	0.2	-0.1

#### 4.1.4. Appendix X2

Appendix X2 of ASTM E1921-21 describes a data set consisting of six 1/2TC(T) specimens of A533B steel, all tested at -75 °C, which doesn't contain any censored data.

Table 4 compares the results of the analyses reported in E1921-21 and obtained from the NIST spreadsheet “*ASTM E1921 - Homogeneous analysis + screening + simplified method.xlsm*”.

Table 4 - Comparison between ASTM E1921-21 Appendix X2 and NIST software results.

Parameter Analysis	$N$	$r$	$K_o$ (MPa√m)	$K_{Jc(med)}$ (MPa√m)	$T_o$ (°C)
ASTM E1921-21	6	6	115.8	107.2	-80.1
NIST software	6	6	115.4	107.1	-80.1
Difference ASTM/NIST	0	0	0.4	0.1	0.0

#### 4.1.5. Appendix X3

Appendix X3 of ASTM E1921-21 presents a combined data set consisting of 1/2TC(T) specimens and 1TSE(B) specimens (with  $W/B = 2$ ) of A533B steel, tested at multiple temperatures between -130 °C and 23 °C, all with  $a_o/W = 0.5$ . Yield strength and elastic modulus values are provided for some, but not all, temperatures in the test range.<sup>19</sup>

Table 5 compares the results of the analyses reported in E1921-21 and obtained from the NIST spreadsheet “*ASTM E1921 - Homogeneous analysis + screening + simplified method.xlsm*”.

Table 5 - Comparison between ASTM E1921-21 Appendix X3 and NIST software results.

Parameter Analysis	$N$	$r$	$\sum r_i n_i$	$T_o$ (°C)
ASTM E1921-21	53	49	8.1	-48.1
NIST software	53	49	8.0	-48.1
Difference ASTM/NIST	0	0	0.1	0.0

#### 4.1.6. Appendix X5, Section X5.5.1

The example problem presented in Section X5.5.1 corresponds to the tests performed at -55 °C from the data set of Appendix X3 (see 4.1.5 above). This amounts to 16 tests on 1/TC(T) specimens, none of which require censoring.

<sup>19</sup> In other words, some fracture toughness tests were performed at temperatures for which tensile data are not directly available. At these temperatures, linear interpolation is required between the yield strength values provided, while elastic modulus values are obtained from eq. (1).

The results of the homogeneous analysis are compared in Table 6 for E1921-21 and the NIST software.

Table 6 - Comparison between ASTM E1921-21 Section X5.5.1 and NIST software results (homogeneous analysis).

Parameter Analysis	$N$	$r$	$K_o$ (MPa $\sqrt{m}$ )	$K_{Jc(med)}$ (MPa $\sqrt{m}$ )	$T_o$ (°C)
ASTM E1921-21	16	16	100.8	93.5	-49.8
NIST software	16	16	100.5	93.4	-49.8
Difference ASTM/NIST	0	0	0.3	0.1	0.0

Next, the data set is used for the material homogeneity screening evaluation described in section 10.6.3 of ASTM E1921-21. The comparison between ASTM and NIST for this step of the analysis is provided in Table 7.

Table 7 - Comparison between ASTM E1921-21 Section X5.5.1 and NIST software results (homogeneity screening evaluation).

Parameter Analysis	Iteration steps	$T_{oscrn}$ (°C)	$T_{oscrn} - T_{o(step1)}$ (°C)	Screening result
ASTM E1921-21	6	-41.3	8.5	INHOMOGENEOUS
NIST software	6	-41.1	8.7	INHOMOGENEOUS
Difference ASTM/NIST	0	-0.2	-0.2	

Finally, an alternative reference temperature,  $T_{oIN}$ , which accounts for possible material inhomogeneity, is calculated using the simplified method ( $N < 20$ ). The comparison between ASTM and NIST for this step of the analysis is shown in Table 8.

Table 8 - Comparison between ASTM E1921-21 Section X5.5.1 and NIST software results (simplified method).

Parameter Analysis	$T_{omax}$ (°C)	$T_{omax} - T_{oscrn}$ (°C)	$T_{oIN}$ (°C)
ASTM E1921-21	-50.8	-9.5	-41.3
NIST software	-50.8	-9.7	-41.1
Difference ASTM/NIST	0	-0.2	-0.2

## 4.2. Inhomogeneity Evaluation for a Large Data Set ( $N \geq 20$ ) – Appendix X5, Section X5.5.2

Another subset of the Appendix X3 data set, consisting of the 53 specimens tested between -80 °C and 0 °C, is used for the evaluation of material inhomogeneity for a large ( $N \geq 20$ ) data set, using both the bimodal and multimodal evaluation methods. As shown in Appendix X3,  $N = 53$ ,  $r = 49$ , and  $T_o = -48.1$  °C.

### 4.2.1. Material Homogeneity Screening Evaluation: Appendix X5, Section X5.5.2.2

Using the homogeneity screening evaluation of ASTM E1921-21, the results shown and compared in Table 9 for ASTM and NIST were obtained.

Table 9 - Comparison between ASTM E1921-21 Section X5.5.2.2 and NIST software results (homogeneity screening evaluation).

Parameter Analysis	Iteration steps	$T_{oscrn}$ (°C)	$T_{oscrn} - T_{o(step1)}$ (°C)	Screening result
ASTM E1921-21	4	-40.6	7.5	INHOMOGENEOUS
NIST software	4	-40.6	7.5	INHOMOGENEOUS
Difference ASTM/NIST	0	0.0	0.0	

#### 4.2.2. Bimodal Evaluation: Appendix X5, Section X5.5.2.3, Item (1)

A full comparison between the outcome of the bimodal analyses reported in ASTM E1921-21 and obtained from the NIST software is presented in Table 10 (step (a)), Table 11 (step (b)), and Table 12 (step (c)).

Table 10 - Comparison between the results of the bimodal analyses on the data set of Section X5.5.2 from ASTM E1921-21 and NIST software (Section X5.5.2.3, Item (1), step (a)).

Parameter Analysis	$p_A$	$T_A$ (°C)	$T_B$ (°C)	Max[ln(L)]
ASTM E1921-21	0.56	-33.5	-58.0	-243.5
NIST software	0.56	-33.6	-58.1	-243.5
Difference ASTM/NIST	0.00	0.1	0.1	0.0

Table 11 - Comparison between the results of the bimodal analyses on the data set of Section X5.5.2 from ASTM E1921-21 and NIST software (Section X5.5.2.3, Item (1), step (b)).

Parameter Analysis	$\sigma_{pA}$	$\sigma_{TA}$ (°C)	$\sigma_{TB}$ (°C)
ASTM E1921-21	0.066	4.18	3.84
NIST software	0.066	4.18	3.85
Difference ASTM/NIST	0.000	0.00	-0.01

Table 12 - Comparison between the results of the bimodal analyses on the data set of Section X5.5.2 from ASTM E1921-21 and NIST software (Section X5.5.2.3, Item (1), step (c)).

Parameter Analysis	$MLNH$	$MLNH_{ec}$	$MLNH_{conf}$	Evaluation result
ASTM E1921-21	3.53	3.46	85 %	INHOMOGENEOUS
NIST software	3.52	3.44	85 %	INHOMOGENEOUS
Difference ASTM/NIST	0.01	0.02	0 %	

The 5 % and 95 % bimodal tolerance bounds calculated in step (d) of the ASTM E1921-21 analysis and those returned by the NIST software are compared in Figure 19.



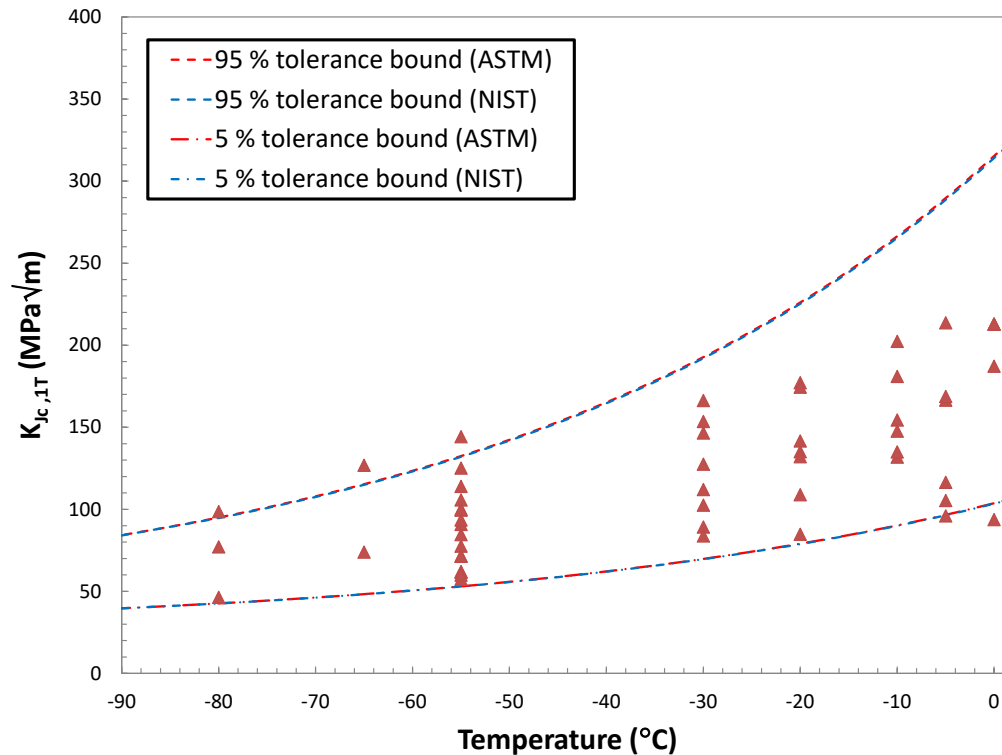


Figure 19 - Comparison between ASTM and NIST bimodal tolerance bounds corresponding to 5 % and 95 % failure probability (data set from Section 5.5.2.2 of E1921-21).

#### 4.2.3. Multimodal Evaluation: Appendix X5, Section X5.5.2.3, Item (2)

A full comparison between the outcome of the multimodal analyses reported in ASTM E1921-21 and obtained from the NIST software is presented in Table 13 (step (a)) and Table 14 (step (b)).

Table 13 - Comparison between the results of the multimodal analyses on the data set of Section X5.5.2 from ASTM E1921-21 and NIST software (Section X5.5.2.3, Item (2), step (a)).

Parameter Analysis	$T_m$ (°C)	$\sigma_{Tm}$ (°C)	Max[ln(L)]
ASTM E1921-21	-43.9	13.2	-243.5
NIST software	-43.8	13.2	-243.4
Difference ASTM/NIST	-0.1	0.0	-0.1

Table 14 - Comparison between the results of the multimodal analyses on the data set of Section X5.5.2 from ASTM E1921-21 and NIST software (Section X5.5.2.3, Item (2), step (b)).

Parameter Analysis	$MLNH$	$MLNH_{conf}$	Evaluation result
ASTM E1921-21	2.77	75 %	INHOMOGENEOUS
NIST software	2.77	74 %	INHOMOGENEOUS
Difference ASTM/NIST	0.00	1 %	

The 5 % and 95 % bimodal tolerance bounds calculated in step (c) of the ASTM E1921-21 analysis and those returned by the NIST software are compared in Figure 20.

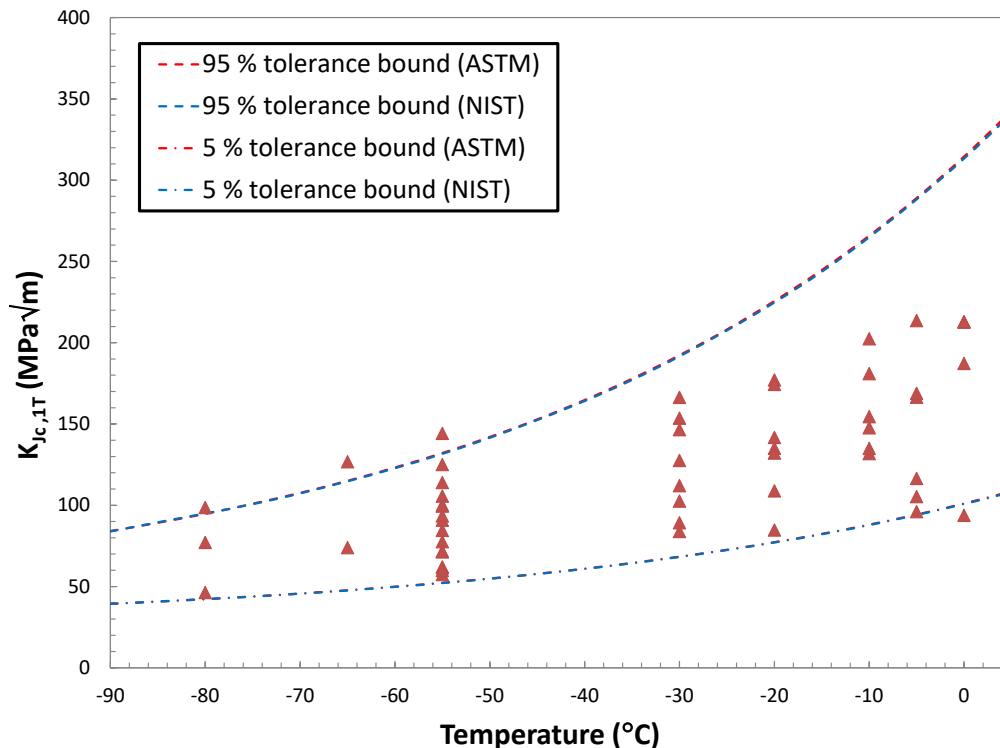


Figure 20 - Comparison between ASTM and NIST multimodal tolerance bounds corresponding to 5 % and 95 % failure probability (data set in Section 5.5.2.2 of E1921-21).

## 5. Conclusions

NIST has developed a macro-enabled, spreadsheet-based software package for the determination of the reference temperature,  $T_0$ , by means of fracture toughness tests performed in the ductile-to-brittle transition region. The analyses to be performed lead to the establishment of the so-called Master Curve, which describes the median fracture toughness  $K_{Jc}$  as a function of test temperature, in accordance with ASTM E1921-21. The assessment of both macroscopically homogeneous and inhomogeneous materials is covered, for both small ( $N < 20$ ) and large ( $N \geq 20$ ) data sets. Detailed instructions for the use of this software were provided in this report.

The NIST software was successfully validated by comparison with several example problems that are provided in appendixes of ASTM E1921-21. The agreement between the output values reported in the ASTM standard and the results obtained from NIST software was found to be excellent:

- For macroscopically homogeneous data sets (seven example problems), the reference temperatures reported by ASTM and NIST coincide within  $\pm 0.1$  °C.
- For the same homogeneous data sets, the largest discrepancies observed were:

- less than  $0.6 \text{ MPa}\sqrt{\text{m}}$  for  $K_o$  (Weibull fitting parameter);
  - less than  $0.2 \text{ MPa}\sqrt{\text{m}}$  for  $K_{Jc,med}$  (median toughness of the data set).
- For a macroscopically inhomogeneous small data set ( $N = 16$ ):
  - $T_{oscrn}$  values (SINTAP approach) differ by  $0.2 \text{ }^\circ\text{C}$ ;
  - the alternative reference temperatures,  $T_{oIN}$ , calculated via the simplified method, differ by  $0.2 \text{ }^\circ\text{C}$ .
- For a macroscopically inhomogeneous large data set ( $N = 53$ ):
  - $T_{oscrn}$  from ASTM and NIST are identical;
  - Bimodal evaluation:
    - $T_A$  and  $T_B$  differ by  $0.1 \text{ }^\circ\text{C}$ ;
    - $p_A$  is identical;
    - $\sigma_{pA}$  and  $\sigma_{TA}$  are identical;
    - $\sigma_{TB}$  values differ by  $0.01 \text{ }^\circ\text{C}$ ;
    - $MLNH$  values differ by  $0.01$ ,  $MLNH_{ec}$  by  $0.02$ , and  $MLNH_{conf}$  is the same;
    - the  $5 \%$  and  $95 \%$  tolerance bounds are in extremely close agreement.
  - Multimodal evaluation:
    - values of  $T_m$  differ by  $0.1 \text{ }^\circ\text{C}$ ;
    - $\sigma_{Tm}$  values are identical;
    - $MLNH$  values are the same, while  $MLNH_{conf}$  differ by  $1 \%$ ;
    - the  $5 \%$  and  $95 \%$  tolerance bounds are in extremely close agreement.

In all cases, the responses about the possible homogeneity or inhomogeneity of the investigated materials were coincident.

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