Main Lab

Calculation Algorithm Validation Worksheet

Summary of Analysis Parameters

for 1664 HEM FOG

on Water

by EPA 1664

This worksheet document validates Element LIMS algorithms that obtain final analytical results from initial values

Laboratory Director: _____

SOP #: _____

Document Control Number: _____

1664 HEM FOG in Water (EPA 1664)

Preservation: Add HCl to pH<2; Store cool at 4°C

Container: Amber Glass - 1000 mL (HCl) **Amount Required:** 1000 **Hold Time:** 10.00 days

Analyte	MDL	Reporting Limit	Surrogate %Rec	Duplicate RPD	Matrix Spike %Rec	Matrix Spike RPD	Blank Spike / LCS %Rec	Blank Spike / LCS RPD
Oil &Grease (HEM)	5	10 mg/L		0.00	15.00-115.00	0.00	15.00-15.00	0.00

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Equation 1: Final Result

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the final result (Rf) in final units:

Equation 1:

$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_s \times F_{Rf}$$

where:

R_f = Final result in final units, rounded to number of significant figures specified on the *Analysis Matrix* dialog

R_i = Initial result in initial data units from the *Data Entry* dialog

F_{Ri} = Unit conversion factor for initial result units

P_f = Preparation final amount from the *Bench Sheet* dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog

F_{Pf} = Unit conversion factor for final preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog

F_{Pi} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog

P_i = Preparation initial amount from the *Bench Sheet* Dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog

S = Solids (Dry Weight). Defaults to 1 (100% Solids) if *Report Dry-Weight Corrected Results* is not checked on the *Analysis Matrix* dialog

D = Dilution factor from *Data Entry* dialog. Defaults to 1

F_s = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected

F_{Rf} = Unit conversion factor for final result units. Note ... if special report units are used, this factor is "1"

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit:

$ppm\ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm\ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm\ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
R_f =		0.00
R_i =		0.00
F_{Ri} =	1.00	
P_f =	0.00	
F_{Pf} =		mg
F_{Pi} =		
P_i =	0.00	ml
S =	1	
D =	0.00	
F_s =	1	
F_{Rf} =	1.00	

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Equation 1: Final Result

Analysis: 1664 HEM FOG **Matrix:** Water

Calculate the final result (Rf) in final units (continued)

Equation 1:

$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_S \times F_{Rf}$$

Use the worksheet below to validate the algorithm used to determine the Final Results:

Rf = ☐ **=** ☐/☐ **X** ☐/☐ **X** ☐/☐ **X** ☐/☐ **X** ☐ **X** ☐ **X** ☐

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Equation 2: Pre-Prep Spike Concentration

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the Spike Concentration (C_f) in final units:

Equation 2:
$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times F_S \times F_{Rf}$$

where:

C_f = Spike level in final units, rounded to number of QC significant figures specified on the *Analysis Matrix* dialog

C_i = Initial concentration of target analyte in the spike mix (ppm)

V = Volume of spike mix added to the sample during preparation, as indicated on the *Bench Sheet* dialog (uL). The 1000 factor is in the equation to convert uL to mL

F_{Pi} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog

P_i = Preparation initial amount from the *Bench Sheet* Dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog

S = Solids (Dry Weight). Defaults to 1 (100% Solids) if *Report Dry-Weight Corrected Results* is not checked on the *Analysis Matrix* dialog

F_S = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected

F_{Rf} = Unit conversion factor for final result units

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit:

$ppm\ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm\ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm\ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
C_f =		mg/L
C_i =		ppm
V =		
F_{Pi} =		
P_i =	0.00	ml
S =	1	
F_S =	1	
F_{Rf} =	1.00	

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Equation 2: Pre-Prep Spike Concentration

Analysis: 1664 HEM FOG **Matrix:** Water

Calculate the Spike Concentration (C_f) in final units (continued)

Equation 2:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times F_S \times F_{Rf}$$

Use the worksheet below to validate the algorithm used to determine the Spike Concentration:

C_f = [ ] = [ ] / [ ] X [ ] X [ ] / [ ] X 1 / [ ] X [ ] X [ ]

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Equation 3: Post-Prep Spike Concentration

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the Spike Concentration (C_f) in final units:

Equation 3:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pf}}{P_f} \times F_{Ri}$$

where:

C_f = Spike level in initial units, rounded to number of QC significant figures specified on the *Analysis Matrix* dialog.

C_i = Initial concentration of target analyte in the spike mix (ppm).

V = Volume of spike mix added to the sample during preparation, as indicated on the *Bench Sheet* dialog (uL). The 1000 factor is in the equation to convert uL to mL.

F_{Pf} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

P_f = Preparation initial amount from the *Bench Sheet* dialog.

F_{Ri} = Unit conversion factor for initial (instrument) result units.

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit:

$ppm\ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm\ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm\ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
C_f =		mg/L
C_i =		ppm
V =		
F_{Pf} =		
P_f =	0.00	ml
F_{Ri} =	1.00	

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Equation 3: Post-Prep Spike Concentration

Analysis: 1664 HEM FOG **Matrix:** Water

Calculate the Spike Concentration (C_f) in final units (continued)

Equation 3:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pf}}{P_f} \times F_{Ri}$$

Use the worksheet below to validate the algorithm used to determine the Spike Concentration:

C_f = [ ] = [ ] / [ ] X [ ] X [ ] / [ ] X [ ]

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Equation 4: Static Spike Concentration

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the Spike Concentration (C_f) in final units:

Equation 4: $$C_f = C_i \times F_{Rf} \times F_S$$

where:

- C_f = Spike level in final units, rounded to number of QC significant figures specified on the *Analysis Matrix* dialog
- C_i = Initial concentration of target analyte in the spike mix (ppm)
- F_{Rf} = Unit conversion factor for final result units
- F_s = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Conversion factors for result units and prep units are necessary to convert them to a ppm value and to a base cgs unit:

$ppm\ (w/v) = \frac{\mu g}{ml}$ in cgs units	$ppm\ (w/w) = \frac{\mu g}{g}$ in cgs units	$ppm\ (v/v) = \frac{nl}{ml}$ in cgs units

Default Values for Analysis Variables:

	Value	Units
C_f =		mg/L
C_i =		ppm
F_{Rf} =	1	
F_s =		

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Equation 4: Static Spike Concentration

Analysis: 1664 HEM FOG **Matrix:** Water

Calculate the Spike Concentration (C_f) in final units (continued)

Equation 4: $$C_f = C_i \times F_{Rf} \times F_S$$

Use the worksheet below to validate the algorithm used to determine the Spike Concentration:

C_f = [ ] **=** [ ] **X** [ ] **X** [ ]

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Equation 5: Pre-Prep Spike Recovery

Analysis: 1664 HEM FOG

Matrix: Water

The following equation calculates the final result % R:

Equation 5: $$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

where:

$\%R$ = Percent Recovery

R_{Spike} = Final result for the spiked sample in final units, unrounded

R_{Source} = Final result for the source sample in final units, unrounded

C_f = Spike level in final units

Note: The final result for the spiked sample and the source sample are calculated using the **Final Results** (Rf) equation see Equation 1

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Below is a three-step calculation worksheet to validate the algorithm % Recovery:

STEP 1: See the following equations to determine the Final Result of the spiked sample and the source sample in final concentration units (see Equation 1)

Step 1 Equation: $$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_S \times F_{Rf}$$

RSpike = ____ = ____ / ____ **X** ____ / ____ **X** ____ / ____ **X** ____ / ____ **X** ____ **X** ____ **X** ____

RSource = ____ = ____ / ____ **X** ____ / ____ **X** ____ / ____ **X** ____ / ____ **X** ____ **X** ____ **X** ____

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Equation 5: Pre-Prep Spike Recovery

Analysis: 1664 HEM FOG

Matrix: Water

Calculates the final result % R using three-step calculation worksheet (continued)

STEP 2: Use the following equation to calculate the Matrix Spike spike concentration:

Step 2 Equation:

$$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times F_S \times F_{Rf}$$

C_f = [ ] **=** [ ] / [1000] **X** [ ] **X** [ ] / [ ] **X** [1] / [ ] **X** [ ] **X** [ ]

STEP 3: Use the values calculated in the first two steps to determine the Matrix Spike % recovery:

Step 3 Equation:

$$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

% R = [ ] **=** ([ ] **–** [ ]) / [ ] **X** [**100**]

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Equation 6: Post-Prep Spike Recovery

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the final result % R:

Equation 6:
$$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

where:

$\%R$ = Percent Recovery

R_{Spike} = Final result for the spiked sample in final units, unrounded

R_{Source} = Final result for the source sample in final units, unrounded

C_f = Spike level in final units

Note: The final result for the spiked sample and the source sample are calculated using the **Final Results** (Rf) equation see Equation 1

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Below is a mulit-step calculation worksheet to validate the algorithm % Recovery:

STEP 1: Determine the Final Result of the spiked sample and the source sample in final concentration units

Step 1 Equation:
$$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_S \times F_{Rf}$$

where:

R_{Source} = The amount of source in the matrix spike in initial concentration units.

P_{iSpike} = Preparation initial amount of the matrix spike from *Bench Sheet* dialog.

$F_{PiSpike}$ = Unit conversion factor for the initial preparation units of the matrix spike. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

$F_{PfSpike}$ = Unit conversion factor for the final preparation units of the matrix spike. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

P_{fSpike} = Preparation final amount of the matrix spike from *Bench Sheet* dialog.

F_{Ri} = Unit conversion factor for the initial concentration units of the matrix spike.

F_{Rf} = Unit conversion factor for the final concentration units of the matrix spike.

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Equation 6: Post-Prep Spike Recovery

Analysis: 1664 HEM FOG **Matrix:** Water

Calculates the final result % R
STEP 1 (continued)

R_f = [ ] = [ ] / [ ] X [ ] / [ ] X [ ] / [ ] X [ ] / [ ] X [ ] X [ ] X [ ]

STEP 2: Calculate the amount of source in the matrix spike in initial concentration units

Step 2 Equation: $$R_{Source} = R_f \times \frac{P_{ispike}}{F_{PiSpike}} \times \frac{F_{PfSpike}}{P_{fSpike}} \times \frac{F_{Ri}}{F_{Rf}}$$

R_{Source} = [ ] = [ ] X [ ] / [ ] X [ ] / [ ] X [ ] / [ ]

STEP 3: Calculate the Final result for the spiked sample in final units, unrounded

Step 3 Equation: $$R_{Spike} = R_i \times D$$

R_{Spike} = [ ] = [ ] X [ ]

STEP 4: Use the following equation to calculate the Matrix Spike spike concentration:

Step 4 Equation: $$C_f = \frac{C_i}{1000} \times V \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times F_S \times F_{Rf}$$

C_f = [ ] = [ ] / 1000 X [ ] X [ ] / [ ] X [ ] / 1 X [ ] X [ ]

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Equation 6: Post-Prep Spike Recovery

Analysis: 1664 HEM FOG

Matrix: Water

Calculates the final result % R
(continued)

STEP 5: Use the valuesfrom equations 1-4 to determine the % Recovery of the Matrix Spike

Step 5 Equation: $$\%\ R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

% R = [ ] **=** [ ] **–** [ ] / [ ] **X** [**100**]

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Equation 7: Static Spike Recovery

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the final result % R:

Equation 7: $$\%R = \frac{R_{Spike} - R_{Source}}{C_f} \times 100$$

where:

$\%R$ = Percent Recovery

R_{Spike} = Final result for the spiked sample in final units, unrounded

R_{Source} = Final result for the source sample in final units, unrounded

C_f = Spike level in final units

Note: Final result for the spiked sample and the source sample are calculated using the **Final Results** (Rf) equation (see Equation 1)

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Below is a multi-step calculation worksheet to validate the algorithm % Recovery:

STEP 1: Determine the Final Result of the spiked sample and the source sample in final concentration units

Step 1 Equation: $$R_f = \frac{R_i}{F_{Ri}} \times \frac{P_f}{F_{Pf}} \times \frac{F_{Pi}}{P_i} \times \frac{1}{S} \times D \times F_S \times F_{Rf}$$

Rf = ☐ = ☐/☐ **X** ☐/☐ **X** ☐/☐ **X** ☐/☐ **X** ☐ **X** ☐ **X** ☐

STEP 2: Calculate the amount of source in the matrix spike in initial concentration units

Step 2 Equation: $$R_{Source} = R_f \times \frac{P_{ispike}}{F_{PiSpike}} \times \frac{F_{PfSpike}}{P_{fSpike}} \times \frac{F_{Ri}}{F_{Rf}}$$

RSource = ☐ = ☐ **X** ☐/☐ **X** ☐/☐ **X** ☐/☐

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Equation 8: Preparation Ratio

Analysis: 1664 HEM FOG

Matrix: Water

The following is the equation used to define the preparation ratio in the event that actual prepation amounts differer from the default values:

Equation 8: $$PR = \frac{\frac{P_i}{P_f}}{\frac{P_{di}}{P_{df}}}$$

where:

PR = Preparation Ratio. Used to adjust the MDL and MRL whtn the actual preparation amounts differ from the default values upon which the normal MDL and MRL are based. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog, or if the percent PR is less than the default *Prep Ratio Threshold* specified in the *Lab Info* dialog.

P_i = Preparation initial amount from *Bench Sheet* dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

P_f = Preparation final amount from *Bench Sheet* dialog. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

P_{di} = Default preparation initial amount from *Analysis Matrix* dialog. If no default is supplied, the actual Preparation Initial amount (P_i) is used.

P_{df} = Default preparation final amount from *Analysis Matrix* dialog. If no default is supplied, the actual Preparation Final amount (P_f) is used.

Note: This equation is used as a variablein *Equation 9: MRL or MDL in final units*

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Use the worksheet below to validate the algorithm used to determine the preparation ratio:

PR= ☐ **=** ☐ **/** ☐ / ☐ **/** ☐

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Equation 9: MDL or MRL in final units

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the final MDL or MRL value in final units, adjusted for preparation variation:

Equation 9:

$$RL_f = \frac{RL_i \times F_S \times D \times F_{Pi} \times F_{Pfd}}{PR \times S \times F_{Pf} \times F_{Pid}}$$

where:

RL_f = Final MDL or MRL in final units, rounded to number of significant figures specified on the *Analysis Matrix* dialog.

RL_i = Initial MDL or MRL in final data units from the *Analysis Matrix* dialog.

F_s = Factor for special reporting units from *Modify Reporting* dialog. Defaults to 1 if no special units have been selected.

D = Dilution factor from *Data Entry* dialog. Defaults to 1.

F_{Pi} = Unit conversion factor for initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

F_{Pfd} = Unit conversion factor for default final preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

PR = Preparation Ratio. Used to adjust the MDL and MRL whtn the actual preparation amounts differ from the default values upon which the normal MDL and MRL are based. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog, or if the percent PR is less than the default *Prep Ratio Threshold* specified in the *Lab Info* dialog.

S = Solids (Dry Weight). Defaults to 1 (100% Solids) if *Report Dry-Weight Corrected Results* is not checked on the *Analysis Matrix* dialog.

F_{Pf} = Unit conversion factor for final preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

F_{Pid} = Unit conversion factor for default initial preparation units. Defaults to 1 if *Use Extraction Initial/Final* is not checked on the *Analysis Matrix* dialog.

Note: This equation is used with the PR variable defined in *Equation 8: Preparation Ration Adjustment*

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Use the worksheet below to validate the algorithm used to determine the Final MDL or MRL:

RLf = [ ] **=** [ ] **X** [ ] **X** [ ] **X** [ ] **X** [ ] / [ ] **X** [ ] **X** [ ] **X** [ ]

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Equation 10: Pre-Prep Spike Recovery

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation calculates the Relative Percent Difference (RPD):

Equation 10: $$RPD = \left| \frac{R_1 - R_2}{R_1 + R_2} \right| \times 200$$

where:

RPD = Relative Percent Difference

R_1 = Final unrounded concentration of the first sample. If *Calculate RPD using %Recovery* is checked on the *Analysis Matrix* dialog, the final unrounded percent recovery value is used when calculating the RPD between spiked samples

R_2 = Final unrounded concentration of the second sample. If *Calculate RPD using %Recovery* is checked on the *Analysis Matrix* dialog, the final unrounded percent recovery value is used when calculating the RPD between spiked samples

Note: Numeric fields use a single precision data type which limit unrounded values to 7 digits of precision

Use the worksheet below to validate the algorithm used to determine the RPD:

RPD = ____ **=** | ____ - ____ / ____ + ____ | **X** 200

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Equation 11: Volume measurement units conversion

Analysis: 1664 HEM FOG **Matrix:** Water

The following equation converts the measurement units of a sample volume from Mass to Volume:

Equation 11: $$R_{v/v} = \frac{R_{m/v} \times F_A \times 1000}{MW}$$

where:

$R_{v/v}$ = Final result in volume/volume units, unrounded.

$R_{m/v}$ = Final result in mass/volume units as calculated using the **Final Results** equation (Equation 1).

F_A = Air Factor specified on the *Lab Info* dialog. Defaults to 24.11 L/Mol.

MW = Molecular Weight of the analyte from the *Analyte* tab of the *Static Lists* dialog.

Use the worksheet below to validate the algorithm used to convert the measurement units from Mass/Volume to Volume/Volume:

$$\mathbf{R_{v/v}} = \square = \frac{\square \times \square \times 1000}{\square}$$

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