A Complete Temperature-Velocity Space Heat Transfer Coefficient Map for Moderator Graphite In The Molten Salt Reactor Experiment

Terry J. Price

Nomenclature

t	Time
h	Heat transfer coefficient
L	Characteristic hydraulic length
k	Thermal conductivity
k_m	Mass transfer coefficient
k_{most}	Mass transfer coefficient for 'most' graphite
$k_{combined}$	Mass transfer coefficient for 'most' and 'central' graphite combined
$k_{central}$	Mass transfer coefficient for 'central' graphite
K_b	Boltzman Constant
Q	Heat
Nu	Nusselt Number
Re	Reynolds Number
Pr	Prandtl Number
x	mixing factor
T	Temperature
f	Function
u	Velocity
D	generic diffusion coefficient / mass diffusion coefficient
H	Fuel channel height

μ   Viscosity

n   Number placeholder

ρ   Density

r_{xe} Xenon atom radius

Introduction

Molten-Salt Reactors (MSRs) are a type of Generation IV nuclear reactor uses a molten alkali-flouride fuel salt to dissolve accidentals into a liquid form . [1] The fluid fuel is circulated between an in core and out of core region.   The fuel salt, when in core, passes through fuel channels which have been cut into a graphite moderator. In this moderating region, the free neutrons become sufficiently thermalized to induce a power producing nuclear chain reaction in the nuclear fuel dissolved in the liquid fuel salt. This nuclear chain reaction imparts heat into the fuel salt and thereby increases the temperature of the salt.   The heated salt then circulates to the out of core region. In this out of core portion of the circulation loop, the fuel salt passes through a heat exchanger which removes energy from the salt and thereby reduces the fuel salt temperature in the process. The cooled fuel salt is then circulated back into the core. Since heat is carried in the fuel salt, this sets up a dynamic in which the fuel salt temperature may be different than the bulk graphite temperature. This can be important in neutronics calculations where the graphite temperature may affect its moderating properties due to Doppler broadening.

The rate heat removal from the salt to the graphite may be described by the equation,

$$\frac{dQ}{dt} = h A \Delta T$$

The heat transfer coefficient (HTC) in this equation, h, may be found through a heat transfer correlations which calculate the Nusselt number (Nu=hL/k) as a function of various dimensionless parameters.

 Typically, forced-convection heat transfer correlations take the form

$$Nu = f\left(\mathrm{Re}, Pr\right) \quad .$$

Reynolds number may be parameterized as a function of flow velocity and temperature,

$$\mathrm{Re} = \mathrm{Re}\left(u, T\right) \quad ,$$

and the Prandtl number may be parameterized as a function of temperature,

$$Pr = Pr(T)$$

Since both the Reynolds number and Prandtl number are parameterized by temperature and velocity, it follows that the Nusselt number and thus the heat transfer coefficient are likewise parameterized by temperature and velocity,

$$Nu = Nu\left(u, T\right) \quad .$$

The Molten Salt Reactor Experiment (MSRE) was an experimental molten salt reactor was built and operated at Oak Ridge National Laboratory (ORNL) in the 1960s. [2] In their 1970 report in Nuclear Science and Engineering, Kerlin and Ball detailed a lumped parameter dynamics model of the MSRE with a 9 node reactor core. In this model, the graphite to fuel-salt heat transfer coefficient of 3.6×10^{-2} MW/K-node is used. [3]

This 9 node model is further expounded upon in ORNL-TM-1070. in which, there mention of two unpublished internal reports that contain information on fuel salt to graphite mass transfer coefficients.. [4] The first report, by O. Burke, described an analog computer simulation of the MSRE which used the same graphite heat transfer coefficient, 3.60×10^{4} W/K-node. It was this HTC from Burke that used in ORNL-TM-1070 dynamics model. In the second unpublished report, by S. Ball, a graphite to fuel salt heat transfer coefficient of 2.43×10^{4} W/K-node was used.

All the graphite to fuel salt HTCs described in these reports are invariant with respect to flow speed and temperature. In a more dynamics analysis, the flow speed and temperature of the fuel-salt vary as transient conditions progress. This work aims to develop a model that predicts heat transfer coefficients as functions of flow speed and temperature for molten salt reactors. In this way, a more detailed transient analysis may be conducted for molten salt reactors, and the MSRE in particular.

Prior Work

The prior work may be briefly broken into two categories, the first as heat transfer coefficients used in performing calculations pertaining to molten salt reactor, and a second category detailing the validation and verification of heat transfer correlations for molten salts from which the heat transfer coefficients are derived.

In the first category, As previously mentioned Kerlin and Ball, in ORNL-TM-1070, used nodal heat transfer coefficients from unpublished sources in their stability analysis of the MSRE. Another report, ORNL-4069, the Dittus-Boelter correlation for heating,

$$Nu = 0.023 \, \mathrm{Re}^{0.8} \, Pr^{0.4} \quad ,$$

was used in a mass transfer analogy to calculate the mass transfer coefficients between the fuel salt and the graphite for xenon. The accuracy of this application of the Dittus Boelter correlation was drawn into question during this investigation since it was found that ORNL-TM-378 reported the MSRE fuel channel Reynolds numbers were between 421 and 3150, [8] yet the range of applicability for the Dittus Boelter correlation is Re > 10^{4}.

In the context of publications pertaining to the validity of heat transfer correlations in molten salt systems, ORNL-TM-4079 by Cooke and Cox investigated forced convection heat transfer measurements in a smooth tube for a molten salt. [5] The heat transfer correlations of Sieder Tate, Martinelli and Boelter, modified Hausen, McAdams, and another correlation by Sieder and Tate were investigated. The report concludes by stating that the results presented averaged 13% below the values

in *standard literature* for heat transfer correlations, and these uncertainties are further compounded by uncertainties in the thermophysical data of the salt.

Finally, a more recent investigation into the applicability of heat transfer correlations was presented by Yoder. [6] In Yoder's paper, experimental heat transfer data in molten salts was compared to predictions by the Seider Tate, a Dittus Boelter like, and Gnielinski correlations. Yoder's report concludes that predictions can be made about heat transfer coefficients using conventional heat transfer correlations for common fluids; however, he also warns that the accuracy of such a prediction is highly dependent on the accuracy of the constituent thermophysical properties used in the calculations.

Methodology

Terminology

UT Space: Velocity, temperature space. The space of potential velocities and temperatures of the system for which a HTC must be generated

Reynolds Map: The Reynolds number evaluated at each point in UT space.

Mark Map: UT space that has been marked with a unique number that identifies the particular HTC to be applied to it.

HTC Map: Heat Transfer Coefficient Map. The value of the heat transfer coefficient marked at each point in UT space.

Overview

In this paper, the MSRE fuel channel was conceptualized as a smooth cylinder with a hydraulic radius equal to the of the non cylindrical fuel channel of the MSRE. The methodology employed herein generates a map of heat transfer coefficients, the HTC map. The HTC map may be viewed as a two dimensional image with a single color channel. Each pixel in the image represents a particular combination of temperature a fuel salt velocity (IE a point in UT space). For this particular HTC map, the range of temperature in UT space are from 750 to 1850K and the velocities range from 0 to 3 m/s.

The first step in the generation of the HTC map is the generation of the Reynolds map. The Reynolds map is a map of Reynolds numbers for each point in UT space. This is important since the Reynolds number is the quantity that determines the applicability of a particular heat transfer correlation.

The applicability of each heat transfer coefficient is evaluated at each point of the Reynolds map and a mask is generated which delineates the regions in which each particular heat transfer coefficient may be evaluated. These masks are each assigned a unique identifier, and each are overlaid on top of a *mark space*. The mark space is not entirely filled by entries from the heat transfer coefficient masks. In particular, the region 2030 < Re < 2300 and the region Re < 13 are devoid of any applicable heat transfer coefficient. Given that the region 2030 < Re < 2300 is much smaller than the range of Reynolds numbers span by the Reynolds space, the *gap* is filled in.

The filling in process uses creates a KD-Tree from the mark space, and subdivides two catagories: those pixels with marks and those pixels without marks. For each of the pixels without marks, its nearest neighbor is found on the KD-Tree of the pixels with marks, and this found nearest neighbor is copied over to the location under inspection.

Although, at this point in the process, the HTC space gives the heat transfer coefficient for every point in UT space, there are jump discontinuities between the different region of heat transfer coefficient applicability. In order to create smooth transitions between the different regions of applicability, the HTC space is conceptualized as a field of scalar quantities to which the diffusion equation,

$$\frac{\partial h}{\partial t} = D \cdot \nabla h \quad ,$$

is applied. The boundary conditions of the diffusion equation are set the Neuman conditions with zero flux penetrating the boundary of the HTC space. The diffusion coefficient is set to 9×10^{-2}, and the space is allowed to diffuse for 2 seconds. Upon completion of this diffusion process, the resultant map gives us a heat transfer coefficient for every potential combination of fuel salt velocity and temperature with smooth transitions between the different heat transfer correlation regions.

Heat Transfer Correlations

Three heat transfer correlations were used to fill the entirety of the UT space. The reader is refered to Tosun for a descrption of these correlations. [8] The first heat transfer correlation is the Sieder Tate correlation for laminar flow,

$$h_1(u, T_{bulk}, T_{wall}) = 1.86 \left(\text{Re}(u, T_{bulk}) \Pr(T_{bulk}) \frac{L}{H} \right)^{1/3} \left(\frac{\mu(T_{bulk})}{\mu(T_{wall})} \right)^{0.14} \frac{k}{L} \quad ,$$

Which is valid in the region 13 < Re <2030. The next correlation is the Whitaker correlation,

$$h_2(u, T_{bulk}, T_{wall}) = 0.015 \, \text{Re}(u, T_{bulk})^{0.83} \, Pr(T_{bulk})^{0.42} \left(\frac{\mu(T_{bulk})}{\mu(T_{wall})} \right)^{0.14} \frac{k}{L} \quad .$$

Which is valid between 2300 < Re < $1 \times 10^{5;}$ however, it is only used up to Re < 1×10^4. For the region above Re > 1×10^4, the Dittus Boelter equation is used,

$$h_3(u, T) = 0.023 \, \text{Re(u,T)}^{4/5} \, Pr(T)^n \frac{k}{L} \quad .$$

Where n is 0.4 if heating, and 0.3 for cooling. A special case where the bulk temperature is the same as the wall temperature is defined such that n=0.35, and this is justified on the fact that Yoder's Dittus Boetler like equation with its n of 1/3 was deemed in good alignment with the experimental data. [7]

The bulk and wall temperatures were taken to be the same in these each of these correlations. This is justified on two points: The first point is as follows:: In all of the previously mentioned correlations, the only place that the difference in bulk and wall temperatures is used is in the ratio of wall to bulk viscosity. In these correlations, the ratio of bulk to wall viscosity is raised to an exponent of 0.14. The

exponent of 0.14 is the smallest exponent on any of the factors in any of the correlations. It follows that the sensitivity of the heat transfer coefficient to variation in the bulk to wall viscosity is smaller than any of the other factors in each of the correlations. The second point is that the temperature of the graphite and the bulk fluid are coupled and near each other in magnitude. In ORNL-TM-0378, the difference in steady state central core fuel salt and graphite temperature was 33 K.[5] Furthermore, the 33 K figure in ORNL-TM-0378 is the bulk graphite temperature, and the wall temperature, as the surface of the bulk temperature, can be expected to be even closer to the bulk fluid temperature. So, given that there is expected to a low sensitivity to changes between bulk and wall temperatures, and the wall and bulk temperatures are coupled. The entire factor,

$$\left(\frac{\mu\left(T_{bulk}\right)}{\mu\left(T_{wall}\right)}\right)^{0.14,}$$

is set to unity. The utility in this is that the entire UT field can be evaluated in terms of a single temperature and velocity parameter. Future work may involve decoupling bulk and wall temperatures.

And so, three heat transfer correlations are used in this work, Sieder Tate, Whitaker, and Dittus Boelter. These correlations are modified so that they can work within the framework of the system under development, however, justifications have been offered for these modifications.

Validation

HTC to HTC Validation

Validation, as succinctly stated by Kapurch "...consists of proof that the system accomplishes (or, more weakly, can accomplish) its *purpose*." [9] In our case, the system is a model which predicts HTCs for MSRs. The *purpose* of model as the prediction of HTCs for MSR fuel channels. Thus, apt validation would be prediction of MSRE fuel salt to graphite heat transfer coefficients such that the predict HTC is congruent with HTCs found in literature.

Given these considerations, first way validation will be performed is through a HTC to HTC validation. The HTCs produced by the technique in this paper are compared to those reported in ORNL reports. Validation is conceptualized as having two constituent components: the predicted (or system generated) data, and the comparison data. The predicted data is that which is produced by the system being validated whereas the comparison data is the data to which the predicted data is compared to.

Given that the aim of this work is to predict the HTC as function of both temperature and fuel-salt velocity, the temperature and fuel-salt velocity at which the validation prediction is to be made is required. According to ORNL-TM-0378, the MSRE had a maximum mid plane fuel salt temperature of 933K and a minimum mid-plane fuel salt temperature of 917K. [5] Furthermore, ORNL-TM-0378 subdivides the MSRE fuel channels into 5 flow regions, summarized in the table below.

Region	Velocity [m/s]
1	0.666

2	0.201
3	0.499
4	0.274
5	0.088

Region 5 will be ignored since it is the annular region between the moderator and the reactor shell. Therefore, the preceding data provide a region of prediction in temperature-velocity space between 913-933K and 0.274 and 0.666 m/s.

ORNL-TM-0728 provides details about the fuel channel dimensions. [10] Fuel channels measure 3.048 × 1.016 cm and have circularly rounded corners. The fuel channel geometry, as depicted in figure 5.7 of ORNL-TM-0728, may be decomposed into 1 rectangle measuring 2.54 ×1.016 cm, and two half circles, each with radii of 0.51 cm. The two half circles are located at the ends of the rectangle. Conceptualizing the geometry as such, the total cross sectional area of a fuel channel is 3.39 cm^2 and there is a perimeter of 10.30 cm. These values give an equivalent hydraulic diameter of 1.32 cm for the MSRE fuel channel.

The variation in fuel-salt thermophysical properties with respect to temperature are not given in the MSRE design report, ORNL-TM-0728; however, a database of temperature dependent thermophysical properties is given in ORNL-2316 (edited by S. Cantor).[7] [10] The fuel salts in ORNL-2316 are denoted F_1-F_4, and each of them have a unique composition. There is an issue, however, in using ORNL-TM-2316 data in that none of the salt mixtures given are identical in composition to the MSRE fuel salt as outlined in ORNL-TM-0728. This discrepancy is solved by choosing fuel salt F_4 in ORNL-2316 to act as an analogue to the MSRE fuel-salt. Justification for this choice will be made by considering the compositions of fuel salt and comparing them to the MSRE fuel salt composition. Under this consideration, in terms of LiF and BeF$_2$ fractions, the composition of salt F_4 is closest, to the partially enriched MSRE fuel salt. Furthermore, since the LiF and BeF$_2$ fractions are the two most significant components of the fuel salt, and as such, the influence of other constituent components are not considered in the determination of the most appropriate analogue.

Another property, the viscosity, as stated in ORNL-TM-2316, of fuel salt F_4 is given by the expression,

$$\mu(T)[kg/m\text{-}s]=(4.44\times10^{-5})\cdot\exp\left(\frac{2086.11}{-255\,T[K]}\right) \quad .$$

The specific heat at constant pressure is invariant for the liquid phase of fuel salt F_4 and is cited as 1381 J/kg-K. The liquid density is given by the expression,

$$\rho(T)[kg/m^3]=3933-1.134\cdot T[K] \quad .$$

The thermal conductivity for F_4 is 0.7 W/m-K and has negligible temperature dependence as justified by the statement,

> "As a first approximation, the temperature dependence of thermal conductivity may be neglected. Although the thermal conductivity of molten salts does vary somewhat with temperature, uncertainties in measurements at a given temperature are usually greater than the temperature dependence over the whole range of temperature.".

The final piece of information used in the validation of the presented technique is the height of the fuel channels. This data is found in ORNL-TM-0728, and is stated as 67" (1.7 m).

Presently, the request data to the HTC calculation has been found. Next, the HTC to which the calculated HTC is to compared is needed. As stated previously, ORNL-TM-1070 provides two heat transfer per node HTCs, 3.6×10^4 W/K-node and 2.43×10^4 W/K-node. [4] Since this work predicts the HTCs on a per unit area basis, these nodal HTCs in literature need to be transformed into areal HTCs.

 ORNL-TM-1070 does not make mention of how much graphite surface area is encapsulated by each node. If, however, as mentioned, in ORNL-4069, a graphite fuel channel surface area of 141 m^2, and, if we assume that the surface area is equally distributed among each of the 9 nodes, then it is calculated that each node has an either areal heat transfer coefficient of either 1.55×10^3 W/m^2-K for the 2.43×10^4 W/K-node value or a HTC 3.23×10^3 W/m^2-K corresponding to the 3.60×10^4 W/K-node value.

In this way, we now have information about the fuel salt thermophysical properties, reactor data, previously determined heat transfer coefficients, and data pertaining to the flow conditions, and this gives us a basis to validate our HTC. All these data will allow us to perform a HTC to HTC comparison for validation.

HTC to MTC Validation

The HTC generated in this paper is also be validated against a mass transfer coefficient (MTC) described in ORNL-TM-3464. [12] This validation is done by using a heat to mass transfer analogy to convert the HTC into a MTC then comparing the converted MTC to a published reference MTC. The conversion process of heat to mass transfer coefficients is described briefly in Annex C of ORNL-4069, and expounded upon more fully by Bergman. [13]Essentially, the process is to replace the Nusselt Number with the Sherwood number and the Prandtl number with the Schmidt number.

In the evaluation of the Sherwood number, the mass diffusion coefficient for xenon in the molten salt is needed. The Einstein-Stokes equation gives a diffusion coefficient for a hard sphere in a liquid, and it is given by,

$$D = \frac{K_b T}{6 \pi \mu(T) r_{xe}} \quad . [14]$$

The radius in the Einstein-Stokes equation is that of a hard sphere with radius equal to that of the diffusing particle. The temperature is taken to be the bulk fuel-salt temperature. The radius of xenon used corresponds to the Xenon van der Waals radius of 216 angstrom, since, by definition, the van der Waals radius is that of an atom conceptulized as a hard sphere. The validity of applying the Einstien Stokes equation to molten salts is discussed by Brockis and Reddy. [15]

The value to which the HTC derived MTC will be compared is fuel salt to graphite mass transfer coefficient for xenon. ORNL-TM-3464 makes mention of a parametric studies in which their MSRE xenon model had its parameters chosen in such a way that the predicted xenon poisoning produced by the xenon model fit the observations from the MSRE xenon observations. The table below summarizes the fuel salt to graphite mass transfer coefficients reported in ORNL-TM-3464.

Region Description in ORNL Report	Value [m/s]
'Most Graphite'	8.47×10^{-7}
'Central Region	5.33×10^{-6}

The predicted mass transfer coefficients are generated as a function of core region as per the discretization in ORNL-TM-0378. The definitions of 'most' and 'central' are not given precisely in the ORNL report. This leads to a mismatch between the discretization of the ORNL report values and the discretization of the values predicted in this report.

This discrepancy is resolved by homogenizing the reported values and the predicted values into a single term. For the predicted values, a weighted average is taken wherein the weights used are derived from the fractional flow rates of each core region. For this comparison, the graphite-shell annuls flow region of the MSRE is ignored since the comparison is between fuel channel MTCs. For the ORNL MTCs, they are combined according to,

$$k_{combined} = (1-x) \cdot k_{central} + x \cdot k_{most} \quad .$$

Where the blending factor, x, is allowed to vary between 0.8 and 0.95 as per a reasonable interpretation of the term 'most'.

Results and Discussion

The the results of the process described in this paper are shown on the *illustration* pages as follow:

- **Frame 1**: The Reynolds map for the MSRE as it was modeled

- **Frame 2**: The masks for each individual HTC

- **Frame 3**: The combined HTC masks

- **Frame 4:** The HTC Mark Mask Regions where no HTC is applicable

- **Frame 5** The filled HTC mark map.

- **Frame 6:** The raw evaluated HTC Map

  - Maximum value → 27805 W/m^2 K.

- **Frame 7:** The Laplacian of the raw HTC Map. The regions where the Laplacian is near zero have been set to white in this plot for clarity.

  - Maximum Value → 10348 W/m^2 K square unit UT Space

- **Frame 8:** The Laplacian of the smoothed HTC Map

  - Maximum Value → 32 W/m^{2}K square unit UT Space

- **Frame 9:** The smoothed HTC Map

  - Maximum Value → 27573 W/m^2 K square unit UT Space

- **Note:** The smoothing operation changed the maximum value by 0.8%, and the laplacian (rate of change) by 99.7%.

- **Frame 10:** MSRE HTC Values found in this work compared to values derived from ORNL-TM-1070 as per the details found in the prior *validation* section.

  - These values are summarized in the table below

Region	Velocity [m/s]	913 K Heat Transfer Coefficient [W/m^2-K]	933 K Heat Transfer Coefficient [W/m^2-K]
	This Work		
1	0.666	908	909
2	0.201	610	609
3	0.499	826	824
4	0.274	676	675
ORNL-TM-1070 Derived Values			

	High Value	1550	Temperature Invariant
	Low Value	2430	

- **Frame 11:** MSRE Fuel Salt to Graphite MTC values found in this work compared to those reported in ORNL-TM-3464.

    ○ These values are summarized below

Region	Velocity [m/s]	913 K Mass Transfer Coefficient [m/s]	933 K Heat Transfer Coefficient [m/s]
This Work			
1	0.666	2.23×10^{-6}	2.43×10^{-6}
2	0.201	1.48×10^{-6}	1.57×10^{-6}
3	0.499	2.01×10^{-6}	2.14×10^{-6}
4	0.274	1.65×10^{-6}	1.77×10^{-6}
ORNL-TM-3464 Reported Values			
'Most Graphite'		8.47×10^{-7}	Temperature Invariant
'Central Region		5.33×10^{-6}	

The mean of the values found in this work is 696 W/m^2-K. Assuming the means by which he areal HTC is determined is correct, this value is lower than the values derived from the ORNL reports by factors of 2.2 and 3.5 respectively.

When weighted by the fractional flow rate for each region, and evaluated at a mean temperature of 924 K, a predicted flow rate weighted MTC of 1.68×10^{-6} is arrived at.   This value is compared to a variable definition of 'most' in **Frame 12**.

Conclusion

The methodology described in this paper generated heat transfer coefficients between fuel-salt and graphite for the MSRE for a range of temperatures and velocities . The HTCs predicted were compared to HTCs derived from ORNL literature. MTCs were generated from these HTCs and compared to MTCs found in ORNL literature

One particular insight into the validity of this technique may be found in MSRE xenon model detailed in ORNL-4069. This xenon model had its parameters fit to experimental data by a bounded random search process.[16] The search found that the fuel salt to graphite mass transfer coefficient that fit the experimental data was lower than the predict mass transfer coefficient by a factor of 6. Given the analogy between mass and heat transfer, although the value of the HTCs predicted in this work are lower than those derived from the ORNL reports, in considering this reduction factor from ORNL-4069

might be considered evidence that the predictions of HTC are more accurate. Of course, a true determination would require an experiment to be performed.