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Cobra-TF Parameter Exposure Work

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<table>
<thead>
<tr>
<th>Revision</th>
<th>Date</th>
<th>Affected Pages</th>
<th>Revision Description</th>
</tr>
</thead>
<tbody>
<tr>
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</table>

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Cobra-TF Parameter Exposure Work

Vincent Mousseau, Noel Belcourt, Robert Salko, Kostadin Ivanov, Maria Avramova, and Mike Doster

September 30, 2014

Abstract

The purpose of this work is to provide improved VUQ capability for CTF. We will initially focus on uncertainty quantification, but we will keep the larger scope of SQA, verification, validation, calibration, and optimization in mind while we work on uncertainty quantification. This is a living document that will be amended as the work is completed. Note that any reference to the CTF software is based on the code version of 12/17/13.

1 The Plan

The plan will consist of the following steps.

1. Initial multipliers for all closure laws in CTF
2. Code multipliers for the Equation Of State (EOS) and material properties
3. Multiplier for the code coupling between CTF and neutronics
4. Specific closure law parameter exposure based on the three PIRTs for VERA-CS progression problem 6, CIPS, and PCI.
5. Location of original journal articles for PIRT identified closure laws
6. Construction of closure law parameter distributions based on the original experimental data that the closure law was based on (expert opinion will supplement when the original data cannot be located).
7. Construction of a parameter input file that CTF will read and DAKOTA can write. Note that this file will be maintained under configuration management and when the default values are read in, there should be no changes to CTF output.
8. Uncertainty quantification of the PIRT parameters with their defined distributions with DAKOTA.

1.1 Steps 1, 2, and 3

This will be the initial phase of the work and it will serve four purposes.

1. An initial fallback position for CTF uncertainty quantification work.
2. Construct a template for all future uncertainty quantification work done by CASL and Penn State.
3. Enable verification work in CTF.

1.1.1 Fallback Position

This initial phase will provide for high level uncertainty quantification for CTF. We already have the ability with DAKOTA to modify CTF input to do uncertainty quantification of CTF initial conditions and boundary conditions (geometry). This new capability will also allow the ability to quantify which closure laws are more or less important to a given Figure Of Merit (FOM) from the PIRT. In addition we will be prepared to address (in a crude fashion) code coupling uncertainties for CTF coupled to neutronics. Finally we will be able to address uncertainty from the equation of state. Although this is far from optimal, it provides a thorough, although high level, uncertainty quantification studies of CTF.
1.1.2 Template

The purpose of this initial work will be to provide a template for future uncertainty quantification work in CTF. As opposed to the traditional methods of either *hard coding* parameter studies or exposing parameters to input, this new approach will provide a maintainable method for building uncertainty capability in the future. In addition, the new approach will also work to minimize the loosely defined, but highly recognized NRC concept of *user effect*. When one adds new parameters to the code input file it provides *nobs* for code users to *tune*. Different code users will *tune* the *nobs* in different ways and this will result in distribution of results. This uncertainty associated with different code users changing the input is called the *user effect*. This new approach for uncertainty quantification will provide a configuration controlled file of the *blessed* parameter values. This configuration control will prevent code users from *tuning* these parameters. The parameter input file will only be modified by DAKOTA. When the parameters are calibrated with experimental data, a new configuration managed parameter file will be created.

1.1.3 Verification

Because of the complexity of the nonlinearly coupled system of equations employed in CTF there are very few exact solutions available for code verification. Since the closure laws embed a large amount of the nonlinearity and most of the coupling between equations, the ability to *turn-off* the closure laws by setting these multipliers to zero, produces a very simplified set of equations. Effectively, one gets three decoupled sets of Euler equations (note the droplet field will be isothermal) and a nonlinear heat conduction equation. A variety of exact solutions are available for these equations.

Many exact equations require a simplified Equation Of State (EOS). Initially by applying multipliers on the input and output of the equation of state, we will be able to simplify this equation. In the future, location of these multipliers will define an *interface* between CTF and the EOS. By cleaning up this interface we will be able to replace the Equation of state in the future with simpler EOSs that lend themselves to analytical solutions. This is left for future work.

1.1.4 Two-phase Model Simplification

The closure laws are what account for almost all of the coupling between the equations. By placing multipliers on the closure laws we can greatly simplify the two phase flow model. By zeroing out all of the droplet coupling terms we reduce down to essentially a six equation model from our initial eight equation model (note thermal equilibrium assumed between droplets and liquid). By then also turning off the interfacial mass momentum and heat transfer we decouple the remaining six equations into two sets of three. This results in a single phase mode.

For the current CASL applications the droplet field is not employed. The ability to simplify the equations should limit unnecessary SQA and UQ testing of the droplet field and should lower memory and improve speed. Zeroing out the appropriate coupling terms is the first step in this direction.

1.2 Step 4

This is where we make the connection to the PIRT and FOM of the challenge problem of interest. There is a bit of work associated with mapping from physical phenomenon identified in the PIRT to closure laws and specific closure law parameters in the CTF software. This work requires a detailed understanding of how physical phenomena are represented in the CTF software. See Appendix A for more detail.

It should be noted here that CTF consists of a variety of closure laws coupled together through some type of logic structure (nested if tests). It is important to not only analyze the uncertainty of the parameters in the closure relations but also to analyze the uncertainty in the parameters that determine when you switch between correlations.

1.3 Step 5

This is where we gather the journal papers that describe the important correlations based on the analysis of the PIRT. The collecting of the original journal papers contributes to the *evidence file* for the problem being studied and for the CTF code. The original journal papers should provide information about the assumptions made in the correlation and the range of applicability. The original journal paper also often contains the experimental data used to develop the correlation. This experimental data can be used for validation of the CTF code. See Appendix B for more detail.
1.4 Step 6

Assuming that we are able to locate the experimental data used to develop the correlation, we can then solve an inverse problem for the distribution of the parameters used in the distribution. This is accomplished by fitting the parameters to the data and the correlation simultaneously. Note that if the original experimental data cannot be found, the parameter ranges will be based on information in the original journal paper and expert opinion.

1.5 Step 7

We need to construct a parameter file that is separate from the input file of CTF. The input file will be employed to study uncertainties in the initial conditions and boundary conditions. There may also be other model flags that switch between competing physical models in the input file. This will be employed to address model error when possible. Based on the above discussion of user effect, the parameters will not be exposed in the CTF input file. A second file that is maintained under configuration management will be employed for uncertainty studies of parameters. This way the pedigree of the code will be maintained by the configuration management of the parameter file. If the parameters are exposed in the input file, there is no way to establish the pedigree of the parameters used in the closure laws in the code.

1.6 Step 8

This step is referred to as a Quantitative PIRT or QPIRT. Here we measure the uncertainty of the Figure Of Merit (FOM) with respect to the parameter distributions. This QPIRT can then be compared to the PIRT. If they both agree on the ranking of phenomena and parameters (note that a one-to-one mapping can be established between parameters and physical phenomena) then we have additional evidence that the PIRT ranking was correct. If the PIRT and QPIRT disagree then this disagreement needs to be resolved by either changing the PIRT, modifying the CTF software, or declaring the discrepancies as acceptable error.

2 Phase I

In the first phase of the work will will focus on steps 1, 7, 8. This will provide the simplest example of how the new uncertainty quantification approach will work. We will start by identifying the conservation equations in CTF and then defining where the code needs to be modified to put a multiplier of the closure law. For software quality checking, if the multiplier is set to one, CTF should produce the same results as the baseline code. If the multiplier is set to zero, the closure law will be turned off and it should be obvious that this physics is no longer active. We are also assuming that smaller perturbations in the parameters around one [0.95, 1.05] should result in small changes in the solution. These three testing strategies will be employed to demonstrate that the new parameters have been implemented correctly.

2.1 Conservation of Mass Closures

The conservation of mass equation for the liquid, vapor, and droplet fields are given below copied from the CTF theory manual.

\[
\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \vec{V}_k) = L_k + M^T_k
\]  

We are only concerned with the non partial differential equation part of this equation which specifically is the right hand side, \(L_k + M^T_k\). It should be noted that the subscript on the M in this equation in the CTF theory manual appears to be incorrectly listed as an e.

The term \(L_k\) accounts for mass change due to boiling and condensation as well as droplet entrainment and deposition (de-entrainment). The term \(M^T_k\) accounts for the mass source and sinks due to turbulent mixing. It is important to note here that turbulence does not create or destroy mass. Velocity gradients may move droplets from a slow channel to a faster channel.

To address the \(M^T_k\) term we will place multipliers in the code in the file vdrift.f near the bottom of the file near line 406 (after the endif and before the 20 continue). There are three variables tmasv, tmasg, and tmasl that will get multipliers added to them.

The \(L_k\) term accounts for creation and destruction of mass between fields. This is partitioned between boiling and condensation, and mass exchange between the droplet and liquid fields caused by droplet entrainment from the liquid field and droplet deposition (de-entrainment) to the liquid field. \(L_k\) is computed from the following formula.
\[ L_v = \Gamma''' \tag{2} \]
\[ L_d = -(1 - \eta)\Gamma'' - S''' \tag{3} \]
\[ L_e = -\eta \Gamma'' + S'' \tag{4} \]

Here \( \Gamma''' \) is the mass transfer rate between vapor and liquid and droplets due to boiling and condensation, \( \eta \) is the partitioning of the boiling and condensation mass transfer between the liquid phase and the droplet phase, and \( S''' \) is the mass transfer due to mechanical forces, entrainment and deposition, between the liquid and droplet field. Note that \( \eta = 0 \) corresponds to no droplets. To control \( L_d \) we need to put multipliers on \( \Gamma''' \), \( \eta \), and \( S''' \).

It is important to note that many of the mass transfer terms are under-relaxed in a variety of ways. When we start the parameter analysis it will be important to catch all of the under-relaxation parameters and test their uncertainty.

Starting with \( \Gamma''' \), this is set in a variable named \texttt{gama} at line 158 of \texttt{Mod_mass_energy_mod.f90}. Next we address \( \eta \) which is set in the file \texttt{infr.f} in the variable \texttt{eta} and the multiplier should be set at line 1370. Finally we have \( S''' \) which is stored in two variables \texttt{sent} and \texttt{sdent} which are set in \texttt{infr.f} near line 1826.

### 2.2 Conservation of Momentum Closures

The conservation of momentum equations are repeated here from the CTF theory manual.

\[
\frac{\partial}{\partial t} \left( \alpha_k \rho_k \vec{V}_k \right) + \frac{\partial}{\partial x} \left( \alpha_k \rho_k u_k \vec{V}_k \right) + \frac{\partial}{\partial y} \left( \alpha_k \rho_k v_k \vec{V}_k \right) + \frac{\partial}{\partial z} \left( \alpha_k \rho_k w_k \vec{V}_k \right) = \alpha_k \rho_k \vec{g} - \alpha_k \nabla P + \vec{\tau}_{wk} + \vec{M}_k^L + \vec{M}_k^d + \vec{M}_k^T \tag{5}
\]

Ignoring the partial differential equation terms and the buoyancy force term we have the following list of closure laws to address, \( \tau_{wk}^T \), \( \dot{M}_k^L \), \( \dot{M}_k^d \), and \( \dot{M}_k^T \). Note that all sheer stress terms are dropped from the momentum equation since they are all accounted for by wall friction, \( \tau_{wk}^T \). Here \( \dot{M}_k^L \) represents momentum source and sinks due to phase change (note that we have already put a multiplier on the phase change so no additional work is required for this term in Phase I), and \( \dot{M}_k^d \) represents interfacial friction, and \( \dot{M}_k^T \) represents momentum transfer due to turbulent mixing.

The wall friction terms, \( \tau_{wk}^T \), are set in \texttt{infr.f} on lines 2186-2188 and are stored in the variables \texttt{xkwwv}, \texttt{xkwlv}, \texttt{xkwev}. The continuous interfacial friction terms, \( \dot{M}_k^d \), are also set in \texttt{infr.f} need to have multipliers applied near line 2186. These variables are stored in \texttt{xl}, \texttt{xkge}, \texttt{xkl}, \texttt{xkle}. The droplet interfacial friction terms are set on line 2428 in \texttt{infr.f} and are stored in \texttt{xkes} and \texttt{xkvl}. The turbulent mixing terms, \( \dot{M}_k^T \), are set in \texttt{vdrift.f} and are stored in \texttt{tmov}, \texttt{tmol}, and \texttt{tmome}. The multipliers for these terms need to be set after the \texttt{endif} and before the \texttt{20 continue} near line 406.

### 2.3 Conservation of Energy Closures

The conservation of energy equation is copied below from the CTF theory manual.

\[
\frac{\partial}{\partial t} (\alpha_k \rho_k h_k) + \nabla \cdot \left( \alpha_k \rho_k h_k \vec{V}_k \right) = -\nabla \cdot \left[ \alpha_k q_k^T \right] + \Gamma_k h_k^i + q_{wk}'' + \alpha_k \frac{\partial P}{\partial t} \tag{6}
\]

Ignoring the partial differential equation terms and the pressure work term and the latent heat released or absorbed (note we already have a multiplier for the mass exchange so this term does not need a new multiplier) we are down to two closure laws, turbulent mixing, \( q_k^T \), and wall heat transfer, \( q_{wk}'' \). We note here that the wall heat transfer terms should be equal and opposite in the wall conduction model. Because there is still some confusion about this we are leaving the wall energy equation out of Phase I.

The turbulent mixing is set in \texttt{vdrift.f} and stored in \texttt{tmrgv} and \texttt{tmrgl}. The multipliers for these terms should be set after the \texttt{endif} and before the \texttt{20 continue} near line 406. The wall heat transfer is set in \texttt{heat.f} and stored in \texttt{qvap} and \texttt{qliq} and the multiplier should be set near line 734. There is also energy transferred from the grid spacer to the vapor field and it is computed in \texttt{infr.f} and stored in \texttt{qvapl} near line 1777.
2.4 Solid Conservation of Energy Closures

The solid transient heat conduction equation is copied below from the CTF theory manual.

\[
(M C_p)_{(i,j,k)} \frac{T_{i,j,k}^{n+1} - T_{i,j,k}^n}{\partial t} = K_{(i,j,k)} \rightarrow (i-1,j,k) \left( T_{i-1,j,k}^{n+1} - T_{i,j,k}^{n+1} \right) \\
+ K_{(i,j,k)} \rightarrow (i+1,j,k) \left( T_{i+1,j,k}^{n+1} - T_{i,j,k}^{n+1} \right) \\
+ K_{(i,j,k)} \rightarrow (i,j-1,k) \left( T_{i,j-1,k}^{n} - T_{i,j,k}^{n} \right) \\
+ K_{(i,j,k)} \rightarrow (i,j+1,k) \left( T_{i+1,j,k}^{n} - T_{i,j,k}^{n} \right) \\
+ K_{(i,j,k)} \rightarrow (i,j,k-1) \left( T_{i,j,k-1}^{n} - T_{i,j,k}^{n} \right) \\
+ K_{(i,j,k)} \rightarrow (i,j,k+1) \left( T_{i+1,j,k}^{n} - T_{i,j,k}^{n} \right) \\
+ Q''_{(i,j,k)} V_{(i,j,k)} 
\] (7)

Here \( M \) is the mass which is input, \( C_p \) is the specific heat which is stored in the variable \texttt{sphst}, and \( K \) is the thermal conductivity which is stored in the variable \texttt{cond}. Because these parameters are computed and used near each other they will be perturbed at the same time.

It should be noted that there is an assumption here that although the density changes with temperature there is an equal and opposite effect on the metal volume keeping the mass constant. However, the metal volume changes without changing the area or the length. This inconsistency should be remembered.

Here the "j" perturbations correspond to axial \texttt{axcon}, and the "k" perturbations correspond to azimuthal \texttt{azcon}.

2.5 List of Parameters that Require Multipliers in Phase I

1. \texttt{eta} Fraction of vapor generation rate coming from the entrained liquid field
2. \texttt{gama} New time vapor generation rate in sub-channel
3. \texttt{sent} Entrainment mass flow rate in sub-channel
4. \texttt{sdent} Deposition mass flow rate in sub-channel
5. \texttt{xtmasv} Loss of mass of vapor in local axial fluid continuity cell due to mixing and void drift to radially adjacent fluid cells
6. \texttt{tmasv} Loss of mass of continuous liquid in local axial fluid continuity cell due to mixing and void drift to radially adjacent fluid cells
7. \texttt{tmasg} Loss of mass of non-condensable gas in local axial fluid continuity cell due to mixing and void drift to radially adjacent fluid cells
8. \texttt{tnomv} Loss of momentum of vapor in sub-channel due to mixing and void drift to radially adjacent fluid cells
9. \texttt{tnome} Loss of momentum of droplets in sub-channel due to mixing and void drift to radially adjacent fluid cells
10. \texttt{tnoml} Loss of momentum of continuous liquid in sub-channel due to mixing and void drift to radially adjacent fluid cells
11. \texttt{xk} Vertical interfacial drag coefficient between the continuous liquid and vapor phases
12. \texttt{xkes} Sink interfacial drag coefficient between the liquid and vapor phases
13. \texttt{xkge} Vertical interfacial drag coefficient between the entrained liquid and vapor phases
14. \texttt{xkl} Transverse interfacial drag coefficient between the continuous liquid and vapor phases
15. \texttt{xkle} Transverse interfacial drag coefficient between the entrained liquid and vapor phases
16. $x_{kvls}$ Sink interfacial drag coefficient between the continuous liquid and vapor phases
17. $x_{kwvw}$ Transverse vapor wall drag coefficient
18. $x_{kwlw}$ Transverse liquid wall drag coefficient
19. $x_{kwvx}$ Vertical vapor wall drag coefficient
20. $x_{kwlx}$ Vertical liquid wall drag coefficient
21. $x_{kwew}$ Transverse entrained liquid form loss coefficient
22. $q_{vapl}$ Incremental heat transferred from grid to vapor
23. $t_{nrgv}$ Loss of enthalpy of vapor in local axial fluid continuity due to mixing and void drift to radially adjacent fluid cells
24. $t_{nrgl}$ Loss of enthalpy of liquid in local axial fluid continuity due to mixing and void drift to radially adjacent fluid cells
25. $r_{odeq}$ Externally supplied heat rate of current rod at current time step (axially averaged)
26. $q_{radd}$ Radiative heat transfer rate from wall to entrained liquid
27. $q_{radv}$ Radiative heat transfer rate from wall to vapor
28. $h_{tcl}$ Liquid heat transfer coefficient
29. $h_{tcv}$ Vapor heat transfer coefficient
30. $q_{liht}$ Heat transfer due to drop impact
31. $s_{phits}$ Specific heat of radial heat transfer
32. $c_{ond}$ Thermal conductivity of radial heat transfer
33. $a_{xcon}$ Axial conductance
34. $a_{zcon}$ Azimuthal conductance
35. $w_{em}$ Lateral momentum of entrained droplet convected by axial velocity
36. $w_{gm}$ Lateral momentum of vapor convected by axial velocity
37. $w_{lm}$ Lateral momentum of liquid convected by axial velocity
38. $c_{dfb}$ Pressure loss coefficient for sub-channel flow blockage
39. $c_{d}$ Pressure loss coefficient of spacer in sub-channel
40. $w_{kr}$ Lateral gap pressure loss coefficient
41. $c_{ool\_avg\_den}$ Average coolant density transferred to coupled neutronics code
42. $c_{ool\_avg\_tmp}$ Average coolant temperature transferred to coupled neutronics code
43. $c_{lad\_avg\_tmp}$ Average clad temperature transferred to coupled neutronics code
44. $c_{fuel\_avg\_tmp}$ Average fuel temperature transferred to coupled neutronics code
45. $h_{gap}$ Gap conductance
3 Parameter Exposure

To provide users with the ability to perturb parameters in CTF, without having to modify the code themselves, we exposed a number of parameters so that they can be set via input files that are automatically looked for, and read if found. This section describes how that parameter exposure work was done, descriptions of parameters that were exposed, how to locate these parameters in the code base along with some discussion about how to expose additional parameters, description of the parameter files, how to use them, and how they interact with both standalone CTF and when CTF is coupled to a neutronics code.

The parameter exposure work was split into two separate capabilities, each with their own, separate, parameter input file. The top-down exposure work focused on identifying PDE closure laws in the mass, momentum and energy equations and applying scalars A and B such that a given closure, x, could toggled on, off or linearly ramped using the scaling Ax+B. The bottom-up exposure work leveraged expert opinion to identify important correlations for the challenge problems of interest, and exposed the various constants present in these important correlations to the user via an input file, so the user could effectively change the correlation without having to change the code. The top-down parameters can be located in the CTF source code by searching for the string "VUQ_PERT", while the bottom-up (correlation) parameters can be found with the string "VUQ_PIRT". By VUQ_PERT, we mean perturbation (closure-law scaling) parameters whereas with VUQ_PIRT, we mean (correlation) parameter importance ranking. In the places where we modified CTF code, you will find one, or both, of these strings indicating the code nearby was modified to support VUQ requirements.

3.1 Top Down Parameters

Top-down parameter exposure work on a scaled closure law Ax+B, permits users to disable the closure (A=0.0, B=0.0), scale the closure (A \neq 1.0) or set the closure to a constant value (A = 0 and B \neq 0) giving good customization capabilities to users. We used a consistent naming convention in the code for how we named closure law multipliers (A) and adders (B). Multipliers are always prefixed with k_ applied to the closure law variable, and likewise for adders, the prefix ka_ is applied to the same closure law variable. For example, cond is the variable name for the thermal conductivity closure, it’s exposed parameters are k_cond and ka_cond so, in the CTF code, you will find an equation of the form:

\[ k_{\text{cond}} \cdot \text{cond}(i, j) + k_{a_{\text{cond}}} \]

3.1.1 Setting Top-Down Parameters via Input File

The user can set the value of the parameters by editing the vuq_mult.txt file. This file currently lists every exposed closure parameter but, because the default for every parameter is already set in the code, this file can be removed or emptied of content and the code will behave the same. The vuq_mult.txt file is located in the CTF source directory (COBRA-TF/cobra_tf/ctf_src) and can be copied into a test directory for setting parameter values. The format of the file is very simple, each line consists of a name = value, one per line. To set a a value, simply add the multiplier or adder value to file with the desired value, for example:

\begin{align*}
  k_{\text{cond}} &= 0.95 \\
  k_{a_{\text{cond}}} &= 0.7
\end{align*}

The order of the values in the file does not matter but the name is case-sensitive and should be lowercase. Note that if a parameter occurs more than once in the file, the last value read from the file will be used and the previous values ignored. If a vuq_mult.txt file is found, a message like this will be output to the console: "Reading VUQ multipliers from vuq_mult.txt". The vuq_mult.txt file should be placed in the same directory as the CTF input deck to ensure it is found when CTF starts up.

3.1.2 Exposing New Closure Parameters

This section describes how you would go about exposing new CTF closure laws. You must first identify the closure variable of interest in the CTF source code. The convention we’ve established is that the multiplier and adder prefix the closure variable as described above. If the closure variable is gravity, you’d be adding two new parameters, k_gravity and ka_gravity. Start by editing the Mod_vuq.f module in the CTF source directory. In the read_multipliers subroutine you’d add a expression for both the multiplier and adder, as you can see for the existing k_cond and ka_cond parameters. You need to add a subroutine in the source file for setting the gravity parameters, called, set_gravity that would be defined in the source file containing the gravity closure law. Note the
use of named parameters in the call to set_cond, this is done so that we write only one single set_cond function that we call multiple times, once for setting the multiplier, once for setting the value of the adder:

```fortran
else if (multiplier.eq.'k_cond') then
call set_cond(mult=value)
else if (multiplier.eq.'ka_cond') then
call set_cond(add=value)
```

Now that the new gravity parameters can be read from the vuq_mult.txt file, you need to implement the set_gravity function in a similar fashion to the set_cond subroutine (Mod_conduction_vuq.f90), reproduced here:

```fortran
subroutine set_cond(mult, add)
  real, optional, intent(in) :: mult, add
  if (present(mult)) k_cond = mult
  if (present(add)) ka_cond = add
end subroutine set_cond
```

Here you can see that we set module variables k_cond and ka_cond to the appropriate value passed into set_cond. You will do something similar in the source code module containing the gravity closure. The last change is to actually scale the gravity closure using the multiplier and adder variables in defined in the module. Here you can see how we scale the conductivity:

```fortran
! VUQ_PERT
kij = k_cond * kij + ka_cond
```

You will do something similar for gravity, and don’t forget to add the comment line with VUQ_PERT as this helps us grep for all the locations of the VUQ modifications in the code base. You will likely have to add some module use declarations so that Mod_vuq.f depends on the module with the gravity closure. Also note that sometimes the same closure occurs in multiple locations in the code base so, in that case, you need to apply the multipliers and adders in multiple places. That should be all that’s needed to expose a new closure to the user.

### 3.2 Bottom Up Parameters

Bottom-up parameter exposure work began with expert opinion identifying the relevant set of correlations thought to dominate the physics in challenge problem 6. The resulting list of correlations were then located in the CTF source code, (see Appendix A) the constants in the correlations identified, and converted into variables whose default value is the correlation default. The default naming scheme for the exposed correlation parameters is to prefix each correlation with k_ followed by the correlation name (if short enough), or an abbreviation, followed by a sequentially increasing number mapping to the various correlation constants. For example, in the case of the Chen correlation, the name scheme is k_chen_1 and k_chen_2 whereas for Dittus-Boelter, we used the abbreviation db so the correlation parameters are numbered k_db_1 through k_db_3 for non-laminar flow. The table below gives the formal name for the correlation, when known so that the short-hand abbreviation can be easily found. Using the Dittus-Boelter correlation as an example, we show both the original correlation and the parameterized version with the exposed variables:

<table>
<thead>
<tr>
<th>Original Equation</th>
<th>Equation with Exposed Parameter</th>
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<tbody>
<tr>
<td>$\text{Nu} = 0.023 \times \text{Re} \quad 0.8 \times \text{Pr} \quad 0.4$</td>
<td>$\text{Nu} = k_{db_1} \times \text{Re} \quad k_{db_2} \times \text{Pr} \quad k_{db_3}$</td>
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</tbody>
</table>

Where the default values for the exposed parameters are as in the original equation.

#### 3.2.1 Setting Bottom-Up Parameters via Input File

The user can set the value of the correlation parameters by editing the vuq_param.txt file. This file has the same format the the vuq_mult.txt file, but can only be used to set the correlation parameters. This file currently lists every exposed correlation parameter but, because the default for every parameter is already set in the code, this file can be removed or emptied of content and the code will behave the same. The vuq_param.txt file is located in the CTF source directory (COBRA-TF/cobra_tf/ctf_src) and can be copied into a test directory for setting correlation parameter values. The format of the file is very simple, each line consists of a name = value, one per line. To
set a a value, simply add the correlation parameter name to the file, with the desired value. For example, to set Dittus-Boelter parameters to use some non-default set of values for some of the parameters, you would add or change these lines in the vuq_param.txt file:

\[
\begin{align*}
  k_{db_1} &= 0.026066218 \\
  k_{db_3} &= 0.35744498
\end{align*}
\]

The order of the values in the file does not matter but the parameter names are case-sensitive and should be lowercase. Whitespace in the file is ignored except that only one parameter can be set per line. If you omit a correlation parameter, the default value of that parameter will be used (i.e. \(k_{db_2}\) is not set in the vuq_param.txt file so it’s value will be 0.8). Note that if a parameter occurs more than once in the file, the last value read from the file will be used and previous values will be ignored (there should probably be a diagnostic message added that warns users that some of the input values are being ignored because they’re set more than once in the file). If a vuq_param.txt file is found, a message like this will be output to the console: "Reading PIRT parameters from vuq_param.txt". The vuq_param.txt file should be placed in the same directory as the CTF input deck to ensure it is found when CTF starts up, just like the vuq_mult.txt file.

### 3.2.2 Adding New Correlation Parameters

This section describes how you would go about exposing new CTF correlation parameters to the user. You would first identify the correlation whose parameters you wish to expose. As described above, the convention we’ve established is that the correlation parameters are prefixed with `k_` followed by the correlation name or abbreviation, followed by a sequential number, one for each parameter in the correlation. Coming up with a meaningful name or abbreviation can be difficult so it’s important to document what you decide to use for the name.

To start with, you’ll need to edit the Mod_vuq.f file and locate the `read_parameters` subroutine. This routine looks for the vuq_param.txt file, reads it and updates the variables listed in the file with the specified values. If a variable listed in the file is not found, an error message like this: "Unknown PIRT parameter in vuq_param.txt", is written to the console and the code is terminated.

We’ll use the Dittus-Boelter (DB) correlation as an example for how we’d expose a new correlation. There are three DB parameters for non-laminar flow, and one additional parameter that is used if the flow is laminar. These values are read from the vuq_param.txt file and set using this code:

```fortran
else if (param .eq. 'k_db_1') then
  call set_db(db1 = value)
else if (param .eq. 'k_db_2') then
  call set_db(db2 = value)
else if (param .eq. 'k_db_3') then
  call set_db(db3 = value)
else if (param .eq. 'k_db_4') then
  call set_db(db4 = value)
```

The variable `param` holds the name read from the input file, likewise for value. Notice how one `set_db` subroutine is called four different ways using named parameters. This helps keep all the code that sets any DB parameter in one subroutine. The `set_db` subroutine is implemented in the module that holds the correlation parameter values, in this case `Mod_DittusBoelter.f90`, as can be seen here:

```fortran
subroutine set_db(db1, db2, db3, db4)
  real, optional, intent(in) :: db1, db2, db3, db4
  if (present(db1)) k_db_1 = db1
  if (present(db2)) k_db_2 = db2
  if (present(db3)) k_db_3 = db3
  if (present(db4)) k_db_4 = db4
  vuq_active = 1
end subroutine set_db
```

Note the use of Fortran named parameters and how one must "ask" if a named parameter was present in the argument list. Also, we set a global variable called `vuq_active` as this flag is used when CTF is coupled to another code, such as a neutronics code (check, this may now be unused). This variable must be set in any subroutine that sets correlation parameters, as you can see above. You will need to add one new `set_correlation` subroutine for each new correlation you expose and you’ll need to add the module dependency to the subroutine that reads the multipliers.
or parameters: For example, this line should be added to both the `read_multipliers` and `read_parameters` subroutines in `Mod_vuq.f` to set the DB parameters:

```fortran
use dittusboelter, only: set_db
```

The last change is to actually modify the correlation to use the exposed parameters instead of the hard-coded constants. Here you can see how we have modified the DB correlation in the `Mod_heatfunctions.f90` file:

```fortran
! VUQ_PIRT
nu = k_db_1 * re ** k_db_2 * pr ** k_db_3
```

Ensure that you add the comment line with VUQ_PIRT as this helps us locate all the PIRT related modifications in the code base.

### 3.2.3 List of Exposed Parameters

This section lists each correlation parameter that can be set via the `vuq_param.txt` input file. Some of the correlations are partially implemented, such as Chen, due to limitations in time or code refactoring that was occurring while this work was being done. In the list that follows, the variable is listed first, followed by its default value, in parenthesis, followed by a description of the correlation the variable is used in.

1. `k_chen_1` (0.24) Chen correlation exponent in: \( dT(w-f)^{0.24} \)
2. `k_chen_2` (0.75) Chen correlation exponent in: \( dP(Tw-Tsat)^{0.75} \)
3. `k_db_1` (0.023) Dittus-Boelter correlation parameter in: \( Nu = 0.023 \times Re^{0.8} \times Pr^{0.4} \)
4. `k_db_2` (0.8) Dittus-Boelter correlation exponent in: \( Nu = 0.023 \times Re^{0.8} \times Pr^{0.4} \)
5. `k_db_3` (0.4) Dittus-Boelter correlation exponent in: \( Nu = 0.023 \times Re^{0.8} \times Pr^{0.4} \)
6. `k_db_4` (7.86) Value of Nu for laminar flow, otherwise Dittus-Boelter correlation is used
7. `k_wf_1` (1.691) Rod wall friction factor
8. `k_wf_2` (0.43) Rod wall friction factor
9. `k_wf_3` (0.117) Rod wall friction factor
10. `k_wf_4` (0.14) Rod wall friction factor
11. `k_wf_5` (0.204) McAdam’s correction parameter in: \( 0.204 \times Re^{-0.2} \)
12. `k_wf_6` (-0.2) McAdam’s correlation parameter in: \( 0.204 \times Re^{-0.2} \)
13. `k_ff_1` (500.0) Interfacial drag coefficients for film flow
14. `k_ff_2` (2.78) Interfacial drag coefficients for film flow
15. `k_ff_3` (2.0) Interfacial drag coefficients for film flow
16. `k_ff_4` (1.6) Interfacial drag coefficients for film flow
17. `k_ff_5` (0.0025) Interfacial drag coefficients for film flow
18. `k_ff_6` (1.0) Interfacial drag coefficients for film flow
19. `k_ff_7` (75.0) Interfacial drag coefficients for film flow
20. `k_ff_8` (4.0) Interfacial drag coefficients for film flow
21. `k_ff_9` (1.53) Interfacial drag coefficients for film flow, hot wall flow regime
22. `k_ff_10` (2.0) Interfacial drag coefficients for film flow, hot wall flow regime
23. `k_ff_11` (0.25) Interfacial drag coefficients for film flow, hot wall flow regime
24. `k_ff_12` (1.252) Interfacial drag coefficients for film flow, hot wall flow regime
25. $k_{bf_1}$ (-2.5) Interfacial drag coefficients for bubbly flow
26. $k_{bf_2}$ (0.4) Interfacial drag coefficients for bubbly flow
27. $k_{bf_3}$ (2.0) Interfacial drag coefficients for bubbly flow
28. $k_{bf_4}$ (24.0) Interfacial drag coefficients for bubbly flow
29. $k_{bf_5}$ (1.0) Interfacial drag coefficients for bubbly flow
30. $k_{bf_6}$ (0.1) Interfacial drag coefficients for bubbly flow
31. $k_{bf_7}$ (0.75) Interfacial drag coefficients for bubbly flow
32. $k_{bf_8}$ (0.4714) Interfacial drag coefficients for bubbly flow
33. $k_{bf_9}$ (2.67) Interfacial drag coefficients for bubbly flow
34. $k_{bf_{10}}$ (0.125) Interfacial drag coefficients for bubbly flow
35. $k_{df_1}$ (0.375) Interfacial drag coefficients for droplet flow
36. $k_{df_2}$ (0.45) Interfacial drag coefficients for droplet flow
37. $k_{cf_1}$ (0.058) Rogers and Rosehart single-phase turbulent mixing coefficient
38. $k_{cf_2}$ (-1.46) Rogers and Rosehart single-phase turbulent mixing coefficient
39. $k_{cf_3}$ (0.5) Rogers and Rosehart single-phase turbulent mixing coefficient
40. $k_{cf_4}$ (-0.1) Rogers and Rosehart single-phase turbulent mixing coefficient
41. $k_{cf_5}$ (1.5) Rogers and Rosehart single-phase turbulent mixing coefficient
42. $k_{cf_6}$ (0.75) Beus’ two-phase turbulent mixing parameter in: $x_0 = 0.75 \times x_{max} \times 0.57 \times re \times 0.0417$
43. $k_{cf_7}$ (0.57) Beus’ two-phase turbulent mixing parameter in: $x_0 = 0.75 \times x_{max} \times 0.57 \times re \times 0.0417$
44. $k_{cf_8}$ (0.0417) Beus’ two-phase turbulent mixing exponent in: $x_0 = 0.75 \times x_{max} \times 0.57 \times re \times 0.0417$
45. $k_{sg_1}$ (0.158) Spacer Grid Enhanced Heat Transfer correlation
46. $k_{sg_2}$ (100.0) Spacer Grid Enhanced Heat Transfer correlation
47. $k_{sg_3}$ (0.25) Spacer Grid Enhanced Heat Transfer correlation
48. $k_{sg_4}$ (0.75) Spacer Grid Enhanced Heat Transfer correlation
49. $k_{sg_5}$ (1.0) Spacer Grid Enhanced Heat Transfer correlation
50. $k_{sg_6}$ (10.0) Spacer Grid Enhanced Heat Transfer correlation
51. $k_{tc_1}$ (2.0) Thom correlation parameter
52. $k_{tc_2}$ (1360.0) Thom correlation parameter
53. $k_{tc_3}$ (72.0) Thom correlation parameter
54. $k_{tc_4}$ (1.0) Thom correlation parameter
55. $k_{tc_5}$ (2.0) Thom correlation parameter
4 Use of Steady State Powers

CTF has the ability to write the steady state powers received from a coupled neutronics code. Typically the power is an input to CTF whereas CTF passes fuel, clad, and coolant temperatures, and coolant density back to the neutronics code. It is occasionally handy to be able to write out the converged neutronics power to a file that can be read into a standalone CTF run, and used as a steady state power profile. For the recent CASL challenge problem, we ran a coupled CTF neutronics problem to steady state convergence and had CTF write the converged power profiles to a file. We were then able to run standalone CTF using the steady state power as a replacement for the coupled neutronics code. In the section below, we describe where the CTF code is that performs these operations and some additional details into it’s use.

In CTF source file Mod_powermod.f90 there are two subroutines that handle reading and writing the steady state power file, read_powers and write_powers. read_powers is called early in CTF so that the power are available to rest of the input processing and a message is written to the console "Reading rodqq power from ss_power.txt" whereas the write_powers routine is called at the very end of the CTF coupled calculation, and this message is written to the console "Writing ss_power.txt". The format of the ss_power.txt is a one line header comment describing the three columns of data to follow, which are: the rod id, the axial level of this rod, and the heat flux in units of BTU/ft^2-sec. This code has not been tested on more than a single assembly so it’s incumbent on the user to test this code before relying on it for multiple assemblies. The write_powers subroutine will only be called at the end of a coupled calculation, it will do nothing if called during a standalone CTF run. If an error is encountered during reading of the steady state powers, this message is written to the console: "Mismatched ss_power.txt and input deck" and usually indicates a power distribution generated from a different CTF core nodalization. Note that the ss_power.txt file should be placed in the same directory as the CTF input deck to ensure it is read during CTF startup.

4.1 Method of Manufactured Solutions

The steady state power profile can be used to support analysis using an MMS type capability. When computing the rod linear power, we can use the perturbation parameters rodqq to perturb the steady state powers read from ss_power.txt. This is done in the mms_rodqq subroutine in Mod_powermod.f90. By default, k_rodqq is 1.0 and ka_rodqq is 0.0 so the steady state powers are not scaled, but they can be by setting these perturbation parameters in the vuq_multi.txt file as described above. Note that if there’s no steady state power input file, the perturbation parameters are applied directly to the rod linearheat array instead of the steady state power.

5 Output VUQ Quantities of Interest

In support of VUQ milestones, we added the ability to output certain quantities of interest (QOI) to VUQ developers. At present we output this data only to the CTF HDF5 file, the following quantities are what’s currently written to the file: maximum fuel, clad, and coolant temperatures along with the assembly, rod, axial, radial, and azimuthal location where the maximum occurred. Temperatures are output in units of degrees Fahrenheit and can be found in the HDF5 by running h5dump and looking for the group labeled QOI. Note that the VUQ QOI group data is written to the HDF5 file only if the code ran in coupled mode (since we require access to data stored in the arrays transferred to the neutronics code), and that there was at least one rod present in the input deck. If both of these conditions were met, then the VUQ data is written to the HDF5 file. Also note that in a coupled calculation, the exact same maximum temperature could occur in multiple locations, the code as written only keeps track of the first location with the maximum temperature. An improvement might list all locations in the core with the peak temperatures.

The code that adds VUQ QOI data to the HDF5 file is in the hdfedit subroutine in Mod_hdfedit.f90 source file. VUQ specific modifications begin around line 180 in this file.

6 Acknowledgements

This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
Appendix A: VERA-CS Progression Problem Six PIRT

Appendix B Uncertainty Library
Thermal Hydraulics
Here we are considering the fluid flow over the fueled portion of the pin.

1. *(H,M)* Subcooled boiling (minimal effect due to void, possible effect due to improved heat transfer but subcooled boiling occurs where the power is low)

### 4.4.6 Sub-Cooled Nucleate Boiling

CTF calculates the heat transfer coefficient in the subcooled nucleate boiling region using Chen correlation:

\[
\hat{h}_{chen} = \hat{h}_{fc} + \hat{h}_{nb}, \quad (4.55)
\]

- Forced Convection Heat Transfer component of the Chen Model

\[
\hat{h}_{fc} = 0.023F_{chen} \left( \frac{k_l}{D_h} \right) Re_t^{0.8} Pr_t^{0.4}, \quad (4.56)
\]

For subcooled nucleate boiling, the F\(_{chen}\) factor is simply equal to 1.

- Nuclear Boiling Heat Transfer coefficient

\[
\hat{h}_{nb} = 0.00122S_{chen} \left( \frac{k_f^{0.79}C_{pf}^{0.45} \mu_f^{0.49} \rho_f^{0.25}}{\sigma^{0.26} \rho_l^{0.24} \rho_g^{0.24}} \right) (T_w - T_f)^{0.24} (P(T_w) - P(T_{sat}))^{0.75}, \quad (4.57)
\]

subroutine htc_chen(dtf,h11,alfl,htcf,dhtc,qnb)

! Uses the Chen correlation to calculate the sub-cooled nucleate boiling and nucleate boiling heat flux and respective heat transfer coefficients.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module</th>
</tr>
</thead>
<tbody>
<tr>
<td>dhtc</td>
<td>Heat transfer coefficient</td>
<td>Mod_htc_models.f boilingf hcoolf heat.f Mod_temp_mod.f</td>
</tr>
<tr>
<td>Variable</td>
<td>Description</td>
<td>Module</td>
</tr>
<tr>
<td>----------</td>
<td>-----------------------------------------------------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>supf</td>
<td>Suppression factor in Chen correlation</td>
<td>Mod_quen.f</td>
</tr>
<tr>
<td>fgama(jh, ns)</td>
<td>Fraction of heat flux that causes sub-cooled boiling at axial heat transfer node jh of rod surface ns</td>
<td>Mod_htcs.f, hcool.f</td>
</tr>
<tr>
<td>fgams(j, ns)</td>
<td>Fraction of heat flux that causes sub-cooled boiling at heat transfer node (= local axial fluid node) j of unheated conductor ns</td>
<td>Mod_htcs.f</td>
</tr>
</tbody>
</table>

2. **(M,H)** Water density (10% change over core uncertainty in steam table ASME 1967 vs. ASME 1998)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rhofl</td>
<td></td>
<td>Blkdat.f</td>
</tr>
</tbody>
</table>

3. **(H,H)** Single phase heat transfer (Dittus Bolter effects fuel temperature)

**4.4.4 Single Phase Vapor Convection**

The Dittus-Boelter correlation

\[
 h_{wv, DB} = 0.023 \frac{k_v}{D_h} Re^{0.8} Pr^n
\]  

(4.51)

The single phase vapor heat transfer coefficient is

\[
 h_{spv} = \frac{k_v}{D_h} Nu_{qh}
\]  

(5.76)
4.4.4 Single Phase Liquid Heat Transfer

The liquid single-phase heat transfer coefficient is

\[ h_{\text{wt}, \text{lam}} = 7.86 \frac{k_l}{D_h} \]  

4. \textbf{(L,M)} Gamma heating (2% of total power directly into the coolant)

5. \textbf{(L,L)} Dimensional changes do to thermal expansion (may be smaller than other uncertainties in thermal hydraulics)

Geometry uncertainty substitute?
6. **(M,M)** Inlet mass flow rate (no feedback from loop so pressure drops sum to zero)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module, subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>GTOT</td>
<td>Total inlet mass flow rate</td>
<td>clearc.f</td>
</tr>
<tr>
<td></td>
<td></td>
<td>dumpit.f</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mod_xtradat.f</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Read_card_1.F90</td>
</tr>
<tr>
<td></td>
<td></td>
<td>restrt.f</td>
</tr>
<tr>
<td></td>
<td></td>
<td>setin.f90</td>
</tr>
<tr>
<td>GINIT</td>
<td>Value of the mass flow rate to initialize mass flow rate in the entire CTF mesh</td>
<td>Read_card_1.F90</td>
</tr>
<tr>
<td></td>
<td></td>
<td>setin.f90</td>
</tr>
</tbody>
</table>

7. **(M,M)** Inlet temperature (no feedback from loop so changes in temperature sum to zero)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module, subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIN</td>
<td>Initial temperature in the fluid domain</td>
<td>If97-bo.f</td>
</tr>
<tr>
<td>HIN</td>
<td>Initial enthalpy in the fluid domain</td>
<td>boiling.f</td>
</tr>
<tr>
<td></td>
<td></td>
<td>clearc.f</td>
</tr>
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<td></td>
<td>cobrai.f</td>
</tr>
<tr>
<td></td>
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<td>dumpit.f</td>
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<td>Mod_setupd.f</td>
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<td>restrt.f</td>
</tr>
<tr>
<td></td>
<td></td>
<td>setout.f</td>
</tr>
</tbody>
</table>
8. (M,H) Wall friction

Rod Friction Factor

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module, subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fv</td>
<td>For vapor</td>
<td>Intrfr.f</td>
</tr>
<tr>
<td>Fl</td>
<td>For liquid</td>
<td>Intrfr.f</td>
</tr>
</tbody>
</table>

Interfacial Drag Coefficient for film flow:

\[
k_{vl} = f_{iw} \rho_v |u_v - u_l| \frac{A_i}{\Delta X}
\]  

(5.40)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module, subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>xkib</td>
<td>Film interfacial drag coefficient</td>
<td>Intrfr.f</td>
</tr>
</tbody>
</table>

Interfacial Drag Coefficient for bubbly flow:

\[
k_{vl,z} = \frac{3}{8} C_{D0} \rho_l |w_{vl} (1 - \alpha_v) L_g \Delta Z_k}{r_b}
\]  

(5.7)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module, subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>xkic</td>
<td>interfacial drag coefficient</td>
<td>Intr.f</td>
</tr>
</tbody>
</table>

Interfacial Drag Coefficient for droplet flow:
9. \textbf{(H,H)} Since our figure of merit is reactivity, we can fix power and do an eigenvalue search (cannot fix eigenvalue = fix reactivity, and do a power search). Until we have transient capability, eigenvalue is the only logical search variable.

10. \textbf{(H,L)} Cross flow models (important near guide tubes)

Turbulent mixing

- the single-phase mixing coefficient, $\beta$, 

Rogers and Rosehart [52] developed correlations for turbulent exchange in bundle geometries. The correlation produces a single-phase mixing coefficient as follows:

$$
\beta_{sp} = 0.5 \lambda Re^{-0.1} \left[ 1 + \left( \frac{D_{h,jj}}{D_{h,ii}} \right)^{1.5} \right] \frac{D_{h,ii}}{D_{rod}}, \text{ if } D_{h,ii} < D_{h,jj} \quad (4.160a)
$$

$$
\beta_{sp} = 0.5 \lambda Re^{-0.1} \left[ 1 + \left( \frac{D_{h,ii}}{D_{h,jj}} \right)^{1.5} \right] \frac{D_{h,jj}}{D_{rod}}, \text{ if } D_{h,jj} < D_{h,ii} \quad (4.160b)
$$

The Beus Correlation provides a mixing coefficient for two-phase flows:

$$
\beta_{tp} = 1 + (\beta_{tp,M} - 1) \left( \frac{x}{x_M} \right), \text{ if } x < x_M \quad (4.162a)
$$

$$
\beta_{tp} = 1 + (\beta_{tp,M} - 1) \left( \frac{x_M - x_0}{x - x_0} \right), \text{ if } x > x_M \quad (4.162b)
$$
11. **(H,M)** Spacer grid model

Grid. f

a. **(H,M)** Loss coefficient is steady state

b. **(M,M)** Mixing term

The mass transport terms due to void drift are:

\[
W_{ij,v}^D = -V_{ij}^T (\alpha_{i,v} \rho_{i,v} + \alpha_{j,v} \rho_{j,v}) (\alpha_i - \alpha_j)_{\text{equil}} S_{ij} \Delta X \\
W_{ij,l}^D = V_{ij}^T (\alpha_{i,l} + \alpha_{j,l}) (\alpha_i - \alpha_j)_{\text{equil}} S_{ij} \Delta X \\
W_{ij,g}^D = -V_{ij}^T (\alpha_{i,g} + \alpha_{j,g}) (\alpha_i - \alpha_j)_{\text{equil}} S_{ij} \Delta X
\] (4.171a)

The momentum void drift terms are:

\[
W_{ij,v}^M = -V_{ij}^T (G_{i,v} + G_{j,v}) (\alpha_i - \alpha_j)_{\text{equil}} S_{ij} \Delta X \\
W_{ij,l}^M = V_{ij}^T \left( \frac{\alpha_{i,l} G_{i,l} + \alpha_{j,l} G_{j,l}}{\alpha_i, l + \alpha_j, l} \right) (\alpha_i - \alpha_j)_{\text{equil}} S_{ij} \Delta X
\] (4.172a)

energy void drift terms are:

\[
W_{ij,v}^H = -V_{ij}^T (\alpha_{i,v} h_{i,v} + \alpha_{j,v} h_{j,v}) (\alpha_i - \alpha_j)_{\text{equil}} S_{ij} \Delta X \\
W_{ij,l}^H = V_{ij}^T (\alpha_{i,l} h_{i,l} + \alpha_{j,l} h_{j,l}) (\alpha_i - \alpha_j)_{\text{equil}} S_{ij} \Delta X
\] (4.173a)
c. **(M,M) Enhanced heat transfer**

The convective heat transfer coefficient is calculated from the film conductivity, the wetted grid surface area, and a two-phase enhancement factor.

\[
h_w = T \frac{k_l}{D_h} Nu A
\]  
(4.139)

The two phase enhancement factor is calculated as follows

\[
T = \min \left[ 10, \sqrt{1 + \frac{0.75 \alpha_e D_h C_d}{D_{df}} \min \left( 1, \frac{(u_e - u_w)}{u_w^2} \right) } \right]
\]  
(4.140)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Module, subroutine</th>
</tr>
</thead>
<tbody>
<tr>
<td>tpenh</td>
<td>Two-phase enhancement of single phase heat transfer coeff</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Intfr.f</td>
</tr>
</tbody>
</table>
Uncertainty Library

March 5, 2014
Contents

1 Heat Transfer Coefficients/Models 3
   1.1 Lee and Ryley ........................................... 3
   1.2 Yuen and Chen ........................................... 3
   1.3 Modified Bromley Correlation ............................. 4
   1.4 Colburn Analogy ......................................... 4
   1.5 Chen Correlation ......................................... 4
   1.6 Thom Correlation ......................................... 5
   1.7 Wong and Hochreiter Correlation ......................... 5
   1.8 Dittus-Boelter ........................................... 6

2 Friction Factor Models 7
   2.1 Wallis Annular flow Interfacial friction correlation ........ 7
   2.2 Henstock and Hanratty .................................... 7
   2.3 Friction Loss Model ....................................... 7

3 Heat Flux Correlations 8
   3.1 W-3 Correlation ........................................... 8
   3.2 Biasi Correlation (Forced Convection Critical Heat Flux) .... 8

4 Mixing Coefficients 9
   4.1 Single Phase Mixing Coefficient ........................... 9

5 Entrainment Models 9

6 Nucleation Temperatures 9
   6.1 Homogeneous Nucleation Temperature (Henry) ............... 9

7 Grid Quench Front Model 10
   7.1 Yamanouchi ............................................... 10

8 Appendix A 10
   8.1 Normal Wall Flow Regimes ................................. 10
      8.1.1 Small Bubble Regime .................................. 10
      8.1.2 Small to Large Bubble Regime ......................... 11
      8.1.3 Churn/Turbulent Flow Regime ......................... 11
      8.1.4 Annular/Mist Flow Regime ............................ 11
   8.2 Hot Wall Flow Regimes .................................... 11
      8.2.1 Inverted Annular Flow ................................ 11
      8.2.2 Dispersed Droplet Flow ............................... 11
      8.2.3 Falling Film Flow .................................... 12
1 Heat Transfer Coefficients/Models

1.1 Lee and Ryley Correlation

\[ h_{i,shl,conv} = \frac{k_f}{D_b} \left( 2.0 + 0.74Re_b^{1/2}Pr_l^{1/3} \right) A_i \]

In Cobra-TF the Lee and Ryley Correlation is used to determine the interfacial heat transfer coefficient for superheated vapor.

- Valid regions in the original paper:
  - Initial Nominal Diameter of the droplet 230 - 1126 microns
  - Droplet Reynolds Number of 64 - 250
  - Degrees of Superheat 5°F - 61°F
  - Steam Pressure 14.7-28.9 psia
  - Steam Velocity 8.8 - 39.2 feet per second
  - Valid for Water

- It should be noted that the 0.74 leading coefficient on the formula from above is higher than the previously determined coefficients from other research papers and the author claims the reason is that previous papers did not consider the vapor as being entirely evaporated into an atmosphere consisting entirely of its own vapor.

- Error Analysis on \( h_{i,shl,conv} = \frac{k_f}{D_b} \left( 2.0 + 0.74Re_b^{1/2}Pr_l^{1/3} \right) \) using figure 5 from Lee and Ryley gives an error of \( \pm 9\% \)

1.2 Yuen and Chen Heat Transfer Coefficient factor

\[ F_{yc} = 1.0 + 0.5 \frac{h_v - h_a}{h_{fg}} \]

In the case of hot wall conditions CTF uses the Lee and Ryley Correlation divided by this factor which has been shown by Yuen and Chen to be necessary at higher temperatures to account for the reduction in heat transfer rates due to evaporation.

- In the original paper of Yuen and Chen the correlation is as follows \( F = 1 + B; \) \( B = \frac{h_v - h_a}{L} \), where \( h_d \) is the enthalpy of the droplet surface and \( L \) is the latent heat of vaporization \( h_{fg} \). Meaning there is an extra 0.5 in the code that is not in the original paper cited by CTF. Not to mention that the code uses a slightly different correlation than is recommended by Yuen and Chen in their paper. The code uses \( h_{i,shl,conv} = \frac{k_f}{D_b} \left( 2.0 + 0.55Re_b^{1/2}Pr_l^{1/3} \right) A_i \), whereas the paper Yuen and Chen recommend \( h_{i,shl,conv} = \frac{k_f}{D_b} \left( 2.0 + 0.6Re_b^{1/2}Pr_l^{1/3} \right) \).

- The correction factor was tested over the following regions
  - \( Re = 200 - 2000 \)
  - Free Stream Air Temperature Range of 150℃ - 960℃
  - Velocity Range of 2.1-11.4 m/s
  - Measured for water and methanol

- Error Analysis on \((1+B)\) using figure 5 from Yuen and Chen original paper gives an error of \( \pm 5.75\% \)
1.3 Modified Bromley Correlation

\[ h_{brom} = 0.62 \left( \frac{D_h}{\lambda} \right)^{0.172} \left[ \frac{k^3_p (\rho_f - \rho_g) H_{fg} g}{D_h \rho_g (T_w - T_{sat})} \right]^{1/4} \]

CTF uses the modified Bromley correlation to calculate the inverted annular film boiling heat flux however the original paper was not developed for this as it was developed and tested for stable film boiling on horizontal tubes.

- CTF uses a modified version of the generally accepted Bromley correlation (As seen in original paper)

- Correlation was developed/tested over the following regions
  - Tested for water, n-Pentane, Benzenem Carbon Tetrachloride, and Ethyl Alcohol
  - \( \Delta t \) ranged from 150°F-2250°F
  - water tested on 0.351 in Carbon Tube
  - Theory is restricted to tubes of such a diameter that the thickness of the film is small compared with the diameter of the tube
  - Horizontal Tubes

- The error associated with the original Bromley Equation is \( \pm 8\% \) from figure 7 in his original paper.

- Does not take into account the \( \left( \frac{D_h}{\lambda} \right)^{0.172} \)

1.4 Colburn Analogy

\[ h_{i,shl,colburn} = f_{HM}(\rho |u_{ul}| |Pr|^{-2/3} A_{i,f} f_{ai} \]

where \( A_{i,f} \) is the interfacial area of the film

- In the original paper one can get the the equation to \( h_{i,shl,colburn} = f_{HM}(\rho |u_{ul}| |Pr|^{-2/3} \) which is close to that CTF uses and it should be noted that this may be as close as the original paper will get as in CTF the \( f_{ai} \) is a ramping factor and the hughmark friction factor is added in on top of this

- The Valid regions for this correlation as quoted by Todreas and Kazimi
  - \( 0.7 < Pr < 100 \)
  - \( Re > 10,000 \)
  - \( L/D > 60 \)

1.5 Chen Correlation

\[ h_{chen} = h_{fc} + h_{nb} \]

\[ h_{fc} = 0.023 F_{chen} \left( \frac{k_i}{\sigma_n} \right) \left( \frac{k_i}{\sigma_n} \right)^{0.8} P_f^{0.4} \] and

\[ h_{nb} = 0.00122 S_{chen} \left( \frac{k_i}{\sigma_n} \right)^{0.79} (\rho C_p g^{0.45} \rho_f g^{0.49} \rho_i g^{0.25}) (T_w - T_f)^{0.24} (P(T_w) - P(T_{sat}))^{0.75} \]

The Chen Correlation is used in the code for the subcooled nucleate boiling region whereas the Correlation was tested over Saturated, Two-Phase Fluid in convective flow. As such the true error may be much more.

- Average Deviation in the Heat Transfer Coefficient according to the paper is \( \pm 12\% \)
  - Tested over Saturated, Two Phase fluid in convective flow
  - Vertical, Axial Flow
  - Stable Flow
  - No Slug Flow
  - No Liquid Deficiency
  - Heat Flux less than CHF
1.6 Thom Correlation

\[ T_{co}(z) = T_{sat} + \zeta^{-1/m} \left( \frac{q''(z)}{10^6} \right)^{1/m} \]

where \( m = 2 \)

\[ \zeta = \frac{\exp \left( \frac{2P}{1260} \right)}{72^2} \]

The initial correlation in the paper given however is

\[ T_s - T_b = \Delta T_{sub} + \Delta T_{sat} \]

where

\[ \Delta T_{sat} = 0.072q''(z)^{1/2} \]

\[ \Delta T_{sub} = T_{sat} - T_b \]

however for the Thom Correlation one can set \( m = 2 \) for the \( \zeta^{-1/m} \left( \frac{q''(z)}{10^6} \right)^{1/m} \) and the following happens

\[ \left( \frac{\exp \left( \frac{2P}{1260} \right)}{72^2} \right)^{-1/2} \left( \frac{q''(z)}{10^6} \right)^{1/2} \Rightarrow \left( \frac{72^2}{\exp \left( \frac{2P}{1260} \right)} \right)^{1/2} \left( \frac{q''(z)^{1/2}}{10^3} \right)^{1/2} \Rightarrow \left( \frac{72}{\exp \left( \frac{P}{1260} \right)} \right) \left( \frac{q''(z)^{1/2}}{10^3} \right) \Rightarrow \left( \frac{0.072q''(z)^{0.5}}{\exp \left( \frac{P}{1260} \right)} \right) = \Delta T_{sat} \]

Now that \( T_{sat} \) has been found if we do some rearrangement of the correlation

\[ T_s - T_b = T_{sat} - T_b + \left( \frac{0.072q''(z)^{0.5}}{\exp \left( \frac{P}{1260} \right)} \right) \Rightarrow T_s = T_{sat} + \left( \frac{0.072q''(z)^{0.5}}{\exp \left( \frac{P}{1260} \right)} \right) \]

which can be rewritten as function of position in the channel

\[ T_{co}(z) = T_{sat} + \zeta^{-1/m} \left( \frac{q''(z)}{10^6} \right)^{1/m} \]

where \( m = 2, P = \text{psia}, q''(z) = \frac{\text{Btu}}{hr*ft^2} \)

- Valid Regions / Tested Regions
  - Pressures between 750-2000 psi
  - water flow rate of 5-20 ft/sec
  - Mass fluxes of 770,000 - 2,800,000 \( \frac{lb}{hr*ft^2} \)
  - Water Inlet subcooling 36-180 °F
  - Heat fluxes between 0-500,000 \( \frac{\text{Btu}}{hr*ft^2} \)

1.7 Wong and Hochreiter Correlation

\[ h_{w,WH} = 0.07907 \frac{k_v}{D_v} Re^{0.6774} Pr_v^{0.333} \]

The Wong and Hochreiter Correlation is an option in the code that might be used in the case of Single-Phase Vapor Convection. In the case of the void fraction being determined to be greater than 0.999 then the Wong Hochreiter Correlation may be selected if it is the maximum of the three correlations used to predict this. Dittus-Boelter and a constant Nusselt-Number value for laminar forced convection being the other two.
Valid Regions

- Developed from ANALYSIS OF THE FLECHT UNBLOCKED BUNDLE STEAM SEASET COOLING (Used heights from 0.61 meters to 1.524 meters because this was steady state in their core)
- Recommended for Pitch to Diameter Ratio of 1.33
- Reynolds Number $2500 \leq Re \leq 25,000$

Error based on report is $Error > 20\% \approx 34\%$ for elevations less than 0.61 meters (not steady state)

Error based on report is $Error < 20\%$ for elevations greater than (0.61 - 1.524) meters

1.8 Dittus-Boelter

- Dittus-Boelter is used in CTF for single phase vapor convection and single phase liquid heat transfer.
- Dittus-Boelter was originally developed for turbulent flow in smooth tubes inside of automobile radiators.
- Valid Regions
  - Inside pipes
  - Prandtl Number $Pr = 0.7 - 120$
  - Reynolds Number $Re = 10,000 - 120,000$
  - Error from figure 3 in original paper is $\pm 15\%$

Initial form of the equation is

$$
\frac{Ud}{k} = 19.5 \left( \frac{dV}{z} \right)^{0.8} \left( \frac{c\eta}{k} \right)^n
$$

where $z = centipoises$, $V = \frac{lb}{ft^2 sec}$, $d = inches$, $c = \frac{Btu}{lb \cdot F}$, $k = \frac{Btu}{hr \cdot ft \cdot F}$

This is not dimensionless, now if we assume an $n$ of 0.4 for heating and convert all the units to make it a dimensionless quantity we get the following

$$
Re = \left( \frac{dV}{z} \right) \frac{1 ft}{12 in} \frac{1 centipoise}{6.7197 \times 10^{-4} \frac{lbm}{ft \cdot sec}}
$$

$$
Pr = \frac{c\eta}{k} \frac{lbm}{ft \cdot hr}
$$

$$
12 Nu = 19.5 \left( 12 \times 6.7197 \times 10^{-4} \right)^{0.8} \left( \frac{1}{2.4191} \right)^{0.4} Re^{0.8} Pr^{0.4}
$$

which leads us extremely close to the common form used today of

$$
Nu = 0.023 Re^{0.8} Pr^m
$$

where $m=0.4$ for heating and $m=0.3$ for cooling
2 Friction Factor Models

2.1 Wallis Annular flow Interfacial friction correlation

\[ f_{sw} = 0.005 \left( 1 + 75 \left( 1 - \alpha_v \right) \right) \]

In CTF the Wallis Annular Flow interfacial friction factor is used as the stable film interfacial friction factor

- Development Ranges
  - For thin film in pipes
  - dimensionless film thickness \(0.001 < \frac{\delta}{D} < 0.04\)
  - Developed for air and water
  - Annular flow

- Error Analysis based on Figure 11.3 in Wallis [72] gives an error of \(\pm 23.72\%\)

2.2 Henstock and Hanratty

\[ f_{sw} = f_s \left( 1 + 1400F \left[ 1 - \exp \left( -\frac{-(1+1400F)^{1.5}}{G_{sw}2p} \right) \right] \right) \]

In CTF the Henstock and Hanratty interfacial friction factor is used as the unstable film interfacial friction factor

- Validity
  - Developed for Downward flow direction
  - Tested for Reynolds number of the liquid flowing in the wall layer between 20-15,100
  - Tested for Reynolds number of the gas between 5,000-112,000

- Error according to of \(\pm 27\%\)

2.3 Friction Loss Model

<table>
<thead>
<tr>
<th>Use</th>
<th>Equation</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Two Phase Pressure Drop</td>
<td>(\frac{dP}{dx\mid_{friction}} = f_{sw}\frac{G_x^2}{\Phi} \Phi^2)</td>
<td>Wallis [72]</td>
</tr>
<tr>
<td>Two Phase Multiplier</td>
<td>(\Phi = 1/\alpha_t), for normal wall conditions</td>
<td>Wallis [72]</td>
</tr>
<tr>
<td>Two Phase Multiplier</td>
<td>(\Phi = 1/\alpha_v), for hot wall conditions</td>
<td>Wallis [72]</td>
</tr>
</tbody>
</table>

The Friction Loss model used above cannot be given an associated error because it is a model and not an empirical fit. However, it should be noted that in Wallis [72], the model from which the two phase multiplier is derived, was intended to be used strictly in Annular flow. As such it is unknown how much error would be incurred by using the above model, with the only way to determine this being to compare it to a model that we can find the error in and see how the above method compares to the known model. It should be noted in the above model that the \(G_x\) is the mass flux of the field of interest.
3 Heat Flux Correlations

3.1 W-3 Correlation

CTF uses the W-3 correlation as an option for determining DNB and critical heat flux.

- Valid Regions according to original paper
  - Pressure \( P = 1000 \text{psia} - 2300 \text{psia} \) (In CTF they claim it is valid down to 800psia)
  - Mass Flux \( G = (1 \times 10^6 - 5 \times 10^6) \text{lbm/hr}\text{ft}^2\)
  - Equivalent Diameter \( D_e = (0.2 - 0.7) \text{inches} \)
  - Quality \( x = (-0.15 - 0.15) \)
  - Inlet Enthalpy \( h_{in} \geq 400 \text{Btu/lbm} \)
  - Length \( L = (10 - 144) \text{inches} \)
  - Valid for either circular tube or rectangular channel geometries
  - Error = uniform and equivalent uniform flux converted from the non-uniform data by using the F-Factor

- Error = \( \pm 20\% \) when the W-3 Correlation is compared with rod bundle DNB data.

3.2 Biasi Correlation (Forced Convection Critical Heat Flux)

- In Cobra TF the Biasi Correlation is used to determine Forced Convection Critical Heat Flux for both low quality and high quality flow.

- Valid Regions
  - Diameter \( D = 0.0030 \text{m} - 0.0375 \text{m} \)
  - Length \( L = 0.2 \text{m} - 6.0 \text{m} \)
  - Pressure \( P = 0.27 \text{MPa} - 14 \text{MPa} \)
  - Mass Flux \( G = 100 \text{kg/m}^2\text{sec} - 6000 \text{kg/m}^2\text{sec} \)
  - Quality \( x = \frac{1}{(1 + \frac{\rho_f}{\rho_g})} - 1 \)

- In the correlation in Cobra TF make sure to input the pressure in bars and not MPa

- Root Mean Square Error (RMS) in biasi is 7.26% and 85.5% of all points are within \( \pm 10\% \)

- For \( G < 300 \text{kg/m}^2\text{sec} \) use equation 4.27a in the code and for \( G > 300 \text{kg/m}^2\text{sec} \) use the larger of the two equations 4.27a and 4.27b
  
  Equation 4.27a) \( q_{b1}'' = 5969500G^{-1/6} [F(P)G^{-1/6} - x] D_h^{n} \)
  
  Equation 4.27b) \( q_{b2}'' = 11980000H(P)(1 - x)D_h^{n}G^{-0.6} \)
4 Mixing Coefficients

4.1 Single Phase Mixing Coefficient

\[ \lambda = 0.0058 \left( \frac{c}{D} \right)^{-1.46} \]

The above equation is used as part of the single phase mixing coefficient for adjacent subchannels

- **Validity**
  - Should only be applied to clean bundles with smooth surfaces
  - \( \frac{c}{D} \) between 0.08-0.4
  - Reynolds Number > 20,000

- According to the paper \( \sigma = 20.8\% \)

5 Entrainment Models

6 Nucleation Temperatures

6.1 Homogeneous Nucleation Temperature (Henry)

\[ T_{min,henry} = T_B + 0.42(T_B - T_l) \left\{ \left( \frac{(k_p C_p)_l}{(k_p C_p)_w} \right) \right\}^{1/2} \left\{ \frac{H_f}{c_p (T_B - T_{sat})} \right\}^{0.6} \]

\[ T_B = T_{sat} + 0.127 \rho_{sat} H_f \frac{g(\rho_f - \rho_g)}{\rho_f - \rho_g} \left( \frac{g(\rho_f - \rho_g) \sigma g}{g(\rho_f - \rho_g) \mu g} \right)^{1/2} \left( \frac{\rho_{sat}}{g(\rho_f - \rho_g)} \right)^{1/3} \]

The above equations are used in the code to help determine the minimum film boiling temperature at which point stable film forms on the heated surface.

- Developed for several different fluids and geometries (Zirconium-Water interactions not being one of them)
- Max Error in Minimum film boiling temperatures of subcooled water 80°F vs 212°F is (+40.9% (stainless steel) to -70.4% (Chrome))
- Max Error in Minimum film boiling temperatures of saturated water (212°F) is (-33.3% (Aluminum)) where -% means the correlation underpredicts and +% means the correlation overpredicts
- Average Error for when the liquid temperature is 212 is +8% and average error for a liquid temperature of 80 degrees is ±28%

Near Wall Condensation Heat Transfer

- The Hancox-Nicoll correlation is used in CTF for near wall heat transfer. Unfortunately Equation 4.61 in CTF was not specifically tested in the original paper rather they used it as a portion of their vapor generation rate equations that they tested.

\[ q''_{hn} = 0.4 \left( \frac{C_p \mu_f D_h}{\mu_f} \right) \left( \frac{G_l D_h}{\mu_f} \right)^{0.662} (T_{sat} - T_l) \]
7 Grid Quench Front Model

7.1 Quench Front Velocity

CTF uses the

\[
V_q = \left[ \frac{\rho_w C_{p,g}}{2} \left( \frac{\delta}{f_{w,g}} \right)^{1/2} \left\{ \left( 1 + 2 \frac{T_g - T_w}{T_w - T_f} \right)^2 - 1 \right\}^{1/2} \right]^{-1}
\]

- Tested over the following regions
  - Channel Flow Rates of 300~1500 \( \frac{kg}{hr} \) and heater flow rates of 1.8~60 \( \frac{kg}{hr} \)
  - Atmospheric pressure
  - Water being the coolant
  - 1500mm long heated rod
- Based on figure 9 in Yamanouchi [77] Error Analysis gave an error of \( \sim 24.8\pm\% \)

Spacer Grid Droplet Breakup Model

- \( \frac{D_{sd}}{D_e} = 6.167W_{ed}^{-0.53} \)
- This is used for determining the diameter of shattered droplets on the spacer grids.

Valid regions and testing notes

- Used if less than 99% of the grid height is quenched
- According to Figure 5.1 in CTF it was tested for \( \sim 60 < W_{ed} < \sim 6000 \)
- For \( W_{ed} < 30.9 \) the large droplet is not considered to enter the small droplet field
- For \( 30.9 < W_{ed} < 250 \) a ramping factor is used
- For \( W_{ed} > 250 \) all large droplets that shatter are considered to enter the small droplet field

- It should be known that the code has a typo in equation 5.111

- Error Analysis on Figure 5.1 in CTF on page 162 gives an approximate Error of \( \pm 23\% \)

8 Appendix A

Flow Regimes have dependence only upon void fraction

8.1 Normal Wall Flow Regimes

8.1.1 Small Bubble Regime

Interfacial area for interfacial drag for small bubbles

\[
A_{i, sb} = 3\alpha_v A_x \frac{\Delta X}{r_b}
\]

Interfacial heat transfer

\[
A_{i, sb} = \frac{6 \max(\alpha_v, 0.001) A_x \Delta X}{D_b}
\]
8.1.2 Small to Large Bubble Regime
code mentions drag correlation but not heat transfer

\[ A_{i,slb} = F_{sb} A_{i,sb} + (1 - F_{sb}) A_{i,lb}^{*} \]

8.1.3 Churn/Turbulent Flow Regime
Interpolation is performed between small to large bubble regime and the annular mist regime for this one using the interpolation factor \( F_a \)

\[ F_a = \frac{\alpha_v - 0.5}{\alpha_{crit} - 0.5} \]

and then the following calculation is done

\[ P_{CT} = F_a P_{AM} + (1 - F_a) P_{SLB} \]

where \( P \) denotes either interfacial drag or interfacial heat transfer where CT, AM, and SLB denotes churn/turbulent, annular/mist, and small-to-large bubble regimes respectively.

8.1.4 Annular/Mist Flow Regime

\[ A_{i,f} = \sqrt{\frac{\alpha^*}{\alpha_v + \alpha_e}} \left( 4\sqrt{\frac{\alpha_v}{\alpha_e}} A_x \Delta X \right) \]

where

\[ \alpha^* = \min \{ 1 - \alpha_i, 1 - \alpha_i(i, j + 1) \} \]

8.2 Hot Wall Flow Regimes
8.2.1 Inverted Annular Flow

\[ A'_{i,f} = 4\sqrt{\alpha_i} A_x \Delta X \]

8.2.2 Dispersed Droplet Flow

\[ A_{i,d} = A'_{i,d} A_x \Delta X \]

where \( A'_{i,d} \) is solved for in the interfacial area transport equation

8.2.3 Falling Film Flow
The falling film regime has both film and vapor

\[ A_{i,f} = \frac{4\sqrt{1 - \alpha_v}}{D_h} \]

and the droplet interfacial area is again solved for in the interfacial area transport equation

\[ A_{i,d} = A''_{i,d} A_x \Delta X \]
8.2.4 Top Deluge Flow

The top deluge regime consists of large liquid slugs

\[ A_{i,s}''' = N_s''' \pi D_s^2 \]

where

\[ N_s''' = \frac{\alpha_l}{\pi D_s^4} \]

and the droplet interfacial area is again solved for in the interfacial area transport equation

\[ A_{i,d} = A_{i,d}''' A_x \Delta X \]