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Verification and Validation of NRC CHF Database & Lookup Table: OECD/NEA Benchmark on CHF AI & ML Phase I

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1. Introduction

In 2019, the U.S. NRC (Nuclear Regulatory Commission), through D.C. Groeneveld, the developer of the critical heat flux lookup table (CHF LUT), publicly released the complete 2006 CHF LUT as well as a database containing 24,579 CHF data points for uniformly heated vertical circular tubes, which were used to develop the CHF LUT [1]. Meanwhile, in 2022, OECD/NEA established a Task Force on Artificial Intelligence and Machine Learning (AI & ML) for Scientific Computing in Nuclear Engineering to develop AI & ML models for benchmark activities. As part of its diverse activities, the Critical Heat Flux Exercise Phase 1 relies on the NRC CHF database for developing CHF AI & ML models, and also considers NRC lookup table as a reference data-driven CHF model [2].

As a preliminary step for the OECD/NEA's ongoing CHF AI & ML Benchmark activities, this study conducted verification and validation (V&V) of NRC CHF LUT based on NRC CHF database. First, we developed a Python subscript for complete 2006 CHF LUT. The developed code was devised to predict CHF not only using the Direct Substitution Method (DSM) but also the Heat Balance Method (HBM). Verification was conducted by evaluating the predictive capabilities of the developed code using the NRC CHF database, and independent validation was performed through comparison with calculation results provided by the OECD/NEA Task Force. Furthermore, parametric trend analysis results were also accumulated to confirm the robustness of the proposed code and the characteristics of CHF in uniformly heated circular tubes. Additionally, the predictive results for CHF were also analyzed using the slicing datasets provided by the OECD/NEA to examine the influence of individual parameters. Finally, differences between DSM and HBM methods were explored, and the causes of predictive differences between the methodologies were reanalyzed.

2. Methods and Results

2.1 NRC CHF LUT

Over the past 70 years, various methods and models have been proposed to predict CHF. Among them, CHF LUT which is a normalized data bank has established itself as a representative data-driven CHF prediction methodology. Recently, the U.S. NRC released the circular tube CHF database used in the development of the NRC lookup table through its author, Groeneveld. Additionally, the complete version of the 2006 Groeneveld CHF LUT, which includes portions that had not been previously published due to space limitations in the Publishing Journal (Nucl. Eng. And Design), was also provided in Appendix III of reference [1]. The newly added section includes intermediate pressure conditions for pressure (P), which are highlighted with underlining, as shown below.

- P [kPa] :
100, 300, 500, 1000, 2000, 3000, <u>4000</u>, 5000, <u>6000</u>, 7000, <u>8000</u>, <u>9000</u>, 10000, <u>11000</u>, 12000, <u>13000</u>, 14000, <u>15000</u>, 16000, <u>17000</u>, 18000, <u>19000</u>, 20000, 21000

The LUT provides CHF values based on pressure, mass flux and quality for a round tube having 8 mm of inner diameter such as

$$q''_{CHF,D=0.008m} = LUT_{DSM}\left(P,G,X\right) \tag{2.1}$$

$$q''_{CHF,DSM} = LUT_{DSM}\left(P,G,X\right)\left(\frac{D}{0.008\,m}\right)^{-0.5} = f\left(P,G,X,D\right) \tag{2.2}$$

Meanwhile, the local thermal equilibrium quality for an uniformly heated channel can be calculated as

$$X = \frac{1}{h_{fg}}\left(h_{in} + \frac{P_h L_h q''_{HB}}{A_c G}\right) - \frac{h_f}{h_{fg}} = \frac{A_h q''_{HB}}{A_c G h_{fg}} - \frac{\Delta h_{in}}{h_{fg}} = \frac{A_h q''_{HB}}{A_c G h_{fg}} + X_{in} \tag{2.3}$$

where q''_{HB} is the channel heat flux satisfying the heat balance equation. When applying Eq. (2.3), CHF correlation can be expressed in terms of inlet condition instead of local condition such as

$$q''_{CHF,DSM} = f\left(P,G,X = \frac{4L}{DG}\frac{q''_{HB}}{h_{fg}} - \frac{\Delta h_{in}}{h_{fg}}, D\right) \quad or \quad f\left(P,G,X = \frac{4L}{DG}\frac{q''_{HB}}{h_{fg}} + X_{in}, D\right) \tag{2.4}$$

In actual heat experiments including CHF condition, heat flux of channel always satisfies with the heat balance equation, however the predicted CHF by correlation (here, LUT DSM on the left-side of Eq.2.4) is not necessarily satisfying. Recalculating CHF based on this satisfaction is the heat balance method (HBM) named by Inasaka and Nariai [3], while Groeneveld referred to this method as calculation under "constant inlet condition" [4]. When assuming $q''_{CHF,DSM} = q''_{HB}$, it leads to an implicit function form such as

$$q''_{CHF,HBM} = f\left(P,G,X = \frac{4L}{DG}\frac{q''_{CHF,HBM}}{h_{fg}} - \frac{\Delta h_{in}}{h_{fg}}, D\right) \quad or \quad f\left(P,G,X = \frac{4L}{DG}\frac{q''_{CHF,HBM}}{h_{fg}} + X_{in}, D\right) \tag{2.5}$$

and generally this can be solved by iterative procedures. Finally the form of correlation based on HBM method can be expressed as

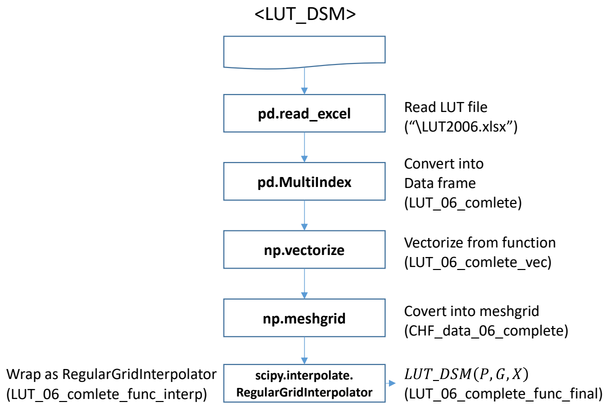
$$q''_{CHF,HBM} = g\left(D, L, P, G, \Delta h_{in} \; or \, T_{in} \; or \; X_{in}\right) \tag{2.6}$$

2.2 Python Code Implementation

A Python library-based code was developed to calculate CHF using the CHF LUT. Since the calculation results vary depending on how the CHF LUT is used, the code was implemented separately for DSM and HBM.

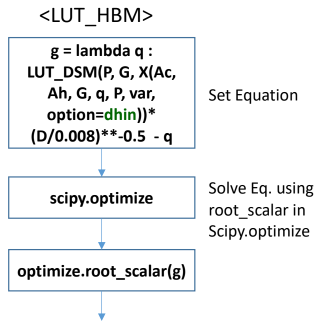
For DSM, the code was designed to load the LUT entries stored in an Excel file and convert them into an object that supports linear interpolation and extrapolation using a Python library (see Figure 1). First, NRC CHF LUT is imported from the file and stored as a single pandas Dataframe object (LUT_06_complete). Then, a function is created to take (*P*, *G*, *X*) as inputs and return the corresponding LUT values from the object (LUT_06_complete_func_final). This function is then vectorized using numpy function (LUT_06_complete_func_vec) and transformed using np.meshgrid to expand the (P, G, X) information into a three-dimensional coddinates (CHF_data_06_complete). Finally, it is converted into a RegularGridInterpolator object from scipy.interpolate, enabling interpolation and extrapolation while returning values as an array based on 3D coordinate data (LUT_06_complete_func_interp). This process results in a function that outputs NRC CHF LUT values (LUT_06_complete_func_final). Since this function only considers (*P*, *G*, *X*), a correction factor for inner diameter (*D* [m]) must be applied to the output to reflect its effect, as shown in Figure 1.

For HBM, considering the inlet subcooling condition, the CHF LUT follows a relationship derived from Eqs. (1.3) and (1.8). Since an implicit function like Equation (2.1) can be numerically solved using the optimize.root_scalar function from the scipy library, the CHF LUT HBM was calculated by constructing a function corresponding to the equation using the previously developed DSM function and solving it numerically (see Figure 2). Additionally, a function was created to compute the quality used as input for the DSM function using heat balance (Eq. (2.3)). This function allows flexibility in input selection through an option variable, enabling calculations based on inlet subcooling (Δh_{in}), inlet temperature (ΔT_{in}), or inlet quality (X_{in}). Consequently, the CHF LUT calculation using HBM also allows different inlet property inputs depending on the selected option. As a result, as discussed in Equation (1.9), the developed CHF LUT HBM function requires five input variables, including the inlet conditions, as illustrated in Figure 2.



$$q''_{CHF,DSM} = LUT\_DSM(P,G,X) \times (D/0.008)^{-0.5}$$

Fig. 1. Python code flow chart –CHF LUT DSM



option=Tin : $q''_{CHF,HBM} = LUT\_HBM(D,L,P,G,T_{in})$

option=Xin : $q''_{CHF,HBM} = LUT\_HBM(D,L,P,G,X_{in})$

option=dhin : $q''_{CHF,HBM} = LUT\_HBM(D,L,P,G,\Delta h_{in})$

Fig. 2. Python code flow chart –CHF LUT HBM

2.3 Code V&V

The predictive performance of the NRC CHF LUT was evaluated not only for the DSM method but also for the HBM method (see Figure 3 and Table I). The performance evaluation utilized all 24,579 data points from the NRC CHF database (N = 24,579). The model performance was evaluated based on the statistical metrics suggested in the CHF AI & ML benchmark for model performance assessment (Table I).

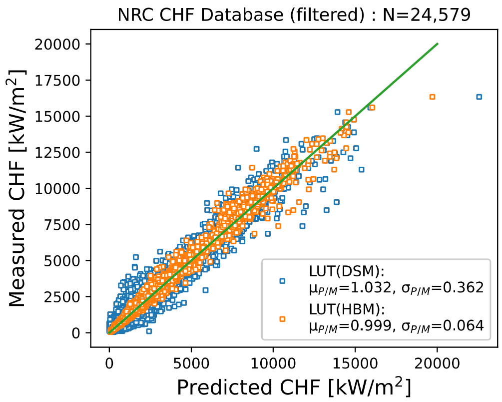


Fig. 3. Code V&V results – NRC CHF LUT (DSM & HBM)

Table I: Problem Description

LUT Method	DSM	HBM
Size of data	24,579	
Mean of P/M	1.032	0.999
Std. of P/M	0.362	0.064
RMSPE [%]	36.30	6.38
MAPE [%]	19.77	4.39
R-squared error	0.941	0.990

As shown in Fig. 3, the mean and standard error of the P/M ratio for the CHF LUT were evaluated as 1.032/0.362 for DSM and 0.999/0.064 for HBM. While there are some differences between the target databases, the RMS Error of the 2006 CHF LUT published in the 2007 reference [4] was reported as 37.21% under fixed local conditions and 5.86% under fixed inlet conditions, which is at a similar level to the present results (see Table 3 in reference [4]).

Meanwhile, the green line in Fig. 3 represents the optimal prediction, where the measured CHF data and the CHF LUT predictions (x, y coordinates) are identical. As observed in the figure, applying the CHF LUT using the HBM method generally exhibits higher predictive performance compared to the DSM method. This can be attributed to the relationship between the critical heat flux model behavior and the thermal equilibrium equation. Further details on this topic are elaborated in Section 2.5.

2.4 Slicing Data Analysis

In the OECD/NEA CHF AI & ML Benchmark, to better understand the influence of individual parameters on CHF, a total of 10 slice datasets were extracted from the NRC CHF database using the slicing method, where measurement conditions were varied for specific parameters only [2]. However, these slice datasets were provided to analyze the trends of CHF data and model predictions solely from a fixed exit condition perspective. Therefore, in this study, to enable comparative analysis with the slicing datasets from a fixed inlet condition perspective as well, additional slicing datasets were newly developed and presented in Table II. Selected results of slicing data analysis from inlet condition perspective are shown in Figs 4-7.

Table II: Slicing Dataset (constant inlet condition)

Slice Set	*D* [mm]	*L* [m]	*P* [kPa]	*G* [kg/m^2/s]	Δh_{in} [kJ/kg]
1	0 ~ 16	6.000	14702	999.0	194
2	0 ~ 16	6.000	9805	1005.0	804
3	8.01	0 ~ 20	9807	1001.0	851
4	8.11	0 ~ 20	2010	751.9	47
5	8.00	1.000	0 ~ 20000	2003.3	305
6	13.40	3.658	0 ~ 20000	2036.5	226
7	8.00	1.570	12750	0 ~ 8000	230
8	10.00	4.966	16000	0 ~ 8000	153
9	8.14	1.943	9832	1519.5	-0.5 ~ 1.0
10	8.00	0.997	17650	2002.7	-0.5 ~ 1.0

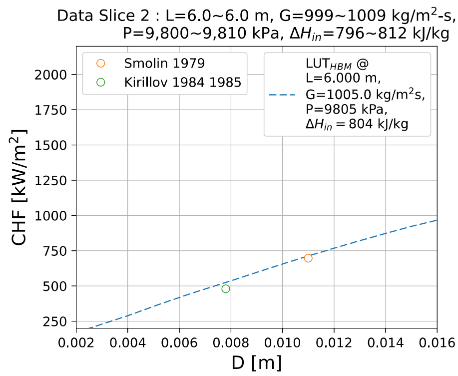


Fig. 4. Sling Data Analysis – *D* effect (Dataset #2)

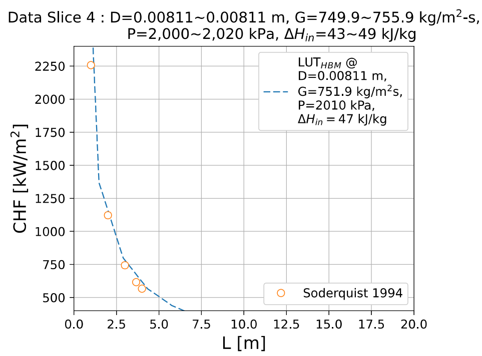


Fig. 5. Sling Data Analysis – *L* effect (Dataset #4)

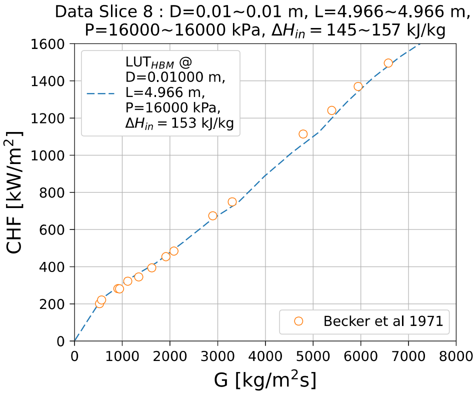


Fig. 6. Sling Data Analysis – Δh_{in} effect (Dataset #6)

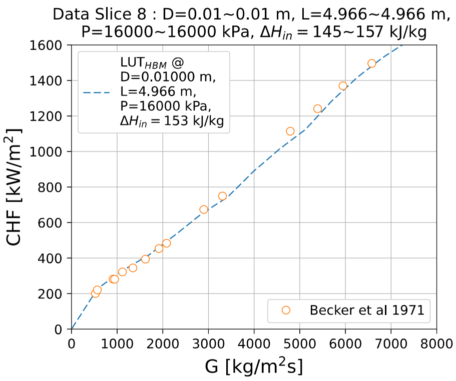


Fig. 7. Sling Data Analysis – G effect (Dataset #8)

2.5 HBM vs DSM

Inasaka and Nariai explained the difference between CHF evaluated using correlations converted to the HBM method and CHF predicted by applying outlet-condition-based correlations in the DSM method through a heat flux–quality graph [3] (Fig. 8). As shown in the figure, outlet-condition CHF correlations generally represent CHF as a decreasing function of quality when all other parameters remain constant, while the thermal equilibrium equation appears as a linear function with a positive slope, as given in Eq. (2.3).

Since uniform heating steady-state experiments always satisfy the heat balance equation, experimental values at any given outlet quality condition exist on the thermal equilibrium. In contrast, CHF predicted by the DSM method using outlet-condition correlations at arbitrary qualities differs from the equilibrium heat flux because the correlation is independent of the thermal equilibrium equation. When the correlation assumes a continuously decreasing function with respect to quality, the intermediate value theorem guarantees that a solution satisfying both equations must exist. This solution, where the correlation and thermal equilibrium equation intersect, represents the HBM heat flux

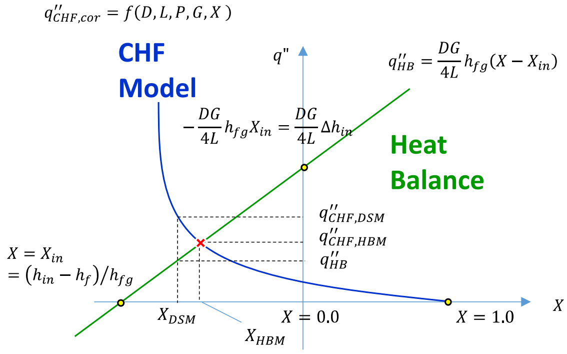


Fig. 8. DSM vs HBM (local condition perspective)

Chang and Baek further developed this discussion, explaining through reference [5] that the predictive capability of the HBM correlation is superior to that of the DSM correlation. As shown in Fig. 8, at any arbitrary point satisfying the thermal equilibrium equation, the following inequality always holds:

$$\left|q''_{CHF,DSM} - q''_{HB}\right| \geq \left|q''_{CHF,HBM} - q''_{HB}\right| \tag{2.7}$$

3. Conclusions

The NRC CHF database and lookup table method serve not only as training and validation data for CHF AI & ML model benchmarking but also as a reference model for data-driven models. Therefore, the contents of this study will be used as reference examples for future CHF AI & ML model development for uniformly heated circular tubes.

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