FORTRAN IMPLEMENTATION FOR NUCLIDE LIQUID DROP MODEL CALCULATIONS WITH NUMERICAL TECHNIQUES

B. Santoso[1], R. Ruliyanta[2]

[1]Department of Physic, Universitas Nasional,
Jl. Sawo Manila, Pasar Minggu, Jakarta, Indonesia.

[2]Department of Electrical Engineering, Universitas Nasional,
Jl. Sawo Manila, Pasar Minggu, Jakarta, Indonesia.

Corresponding Author's Email: [2]ruliyanto@civitas.unas.ac.id

Article History: Received 15 Feb 2025; Revised 25 March 2025; Accepted 15 April 2025

ABSTRACT: This research proposes a numerical variation method developed to find the best parameters of the nuclide liquid drop model in calculating its mass. This method was developed because there was no systematic method for finding empirical model parameters in calculating the nuclide mass or binding energy. The modelling used in this study uses the Fortran programming language or formula translation. The results obtained provide a very significant improvement in the model for calculating the mass of stable nuclides. The closeness of the empirical model calculation results to the experimental results shows the model's validity. The delta deviation results from the proposed numerical method give the smallest value compared to existing methods at 111. Meanwhile, the error rate in the proposed method is 0.00088% or 8.84×10^{-6}.

KEYWORDS: *Numerical; Nuclide; Fortran; Proton; Neutrons*

1.0 INTRODUCTION

The liquid drop model for calculating nuclide binding energies has been developed since 1913 and was first proposed by Bohr [1], [2]. The Bohr model uses many assumptions and approximations to simplify the description of nuclide behaviour. One example is the Bohr model of the hydrogen atom, which only considers one electron, while nuclides have many protons and neutrons that interact in complex ways [3], [4]. The binding energy formulated on a semi-empirical basis by Weizsacker turns out to be sufficient to provide an estimate for knowing the energy balance of various nuclear quantities such as nuclide mass, binding energy, energetic beta decay, alpha decay, nuclear reactions, resonant reaction cross sections and energetic fission [1], [5]. This model has undergone improvements with various choices of model parameters. The empirical model used assumes that the binding energy consists of nucleon binding energy, which is proportional to the mass number A, surface binding energy, considering that liquid drops always have surface energy, Coulomb repulsion energy, which is directly proportional to the atomic number Z squared, symmetry energy to the number of neutrons and protons, and the discrete energy due to nucleons as fermion particles. [1], [5].

This research aims to create a numerical model to calculate nuclide energy so minimal errors occur. [6]. The method assumes that each parameter is referred to sequentially as a1, a2, a3, a4, and a5. Hence, the key is to set the parameters so that the error in the model calculation results compared to experimental data is the smallest. The determination is carried out using a trial system, and it is unclear what the best trial method is to obtain the best parameter values. [7], [8], [9], [10]. The modelling used in this study uses the Fortran programming language or formula translation. The results of the numerical calculations are compared with the parameters that have been tested, including those given by Segre. [11], [12], Elton [13], Kaplan[14], Godfrey [15], Vincent [16], and Keenan [17]. This paper proposes an iterative numerical variation method to obtain the best parameter quantities. [9], [16]. The selection of nuclide data is limited to stable nuclides only.

2.0 METHOD

Nuclides with atomic number Z have Z protons. [18]. The mass number A indicates the presence of A nucleons (protons and neutrons)—the number of nucleons that comprise the nuclide as a constituent with Equation 1.

$$M = Z.M_P + (A - Z).M_N = 1.008983\,A - 0.000839\,Z \quad \text{(1)}$$

The mass of a proton is 1.0081437, and the mass of a neutron is 1.0089830 mass units. However, the mass changes according to the binding energy used because of the negative binding energy. Using the water drop model, the first correction comes from the binding energy of nucleons (protons or neutrons) whose magnitude is proportional to A and is given by Equation 2.

$$M_V = a_{V.}A \quad (2)$$

The constant a1 is a constant that needs to be determined, as are the constants involved in subsequent corrections. This first correction ignores the situation where, at the surface, the nucleon binding energy is smaller. Therefore, it is necessary to provide a surface effect correction, the amount of which is calculated using Equation 3.

$$M_S = a_{S.}A^{2/3} \quad (3)$$

The next correction comes from the mutual repulsion force between protons, which is proportional to *Z(Z*–1). Based on quantum calculations, this energy is only proportional to Z_2, so the correction can be calculated with equation 4.

$$M_C = a_{C.}Z(Z-1)/A^{1/3} \quad (4)$$

For a charge with a uniform distribution, the constant a_3 is 3e2/5.r0 = 0.000763. The last fact shows stability around the position where the number of protons and neutrons equals. This correction is given by equation 5.

$$M_{SY} = a_{SY}(A/2-Z)^2/A \quad (5)$$

All calculated terms show a continuous dependence of the nuclide energy on the number of neutrons and protons. However, some components are still not continuous, namely due to the evenness of A. This energy correction is given by equation 6.

$$D(A, Z) = + a\delta f(A) \quad (6)$$

for A even Z odd, = 0 for A odd and = - aδ f(A) for A even Z odd.

ISSN: 2672-7188 e-ISSN: 2682-8820 Vol. 7 No. 1 2025

Various experts, among others, have established the approach for unknown coefficients, which is given by reference. Next, the form of Equation 7 will be used.

$$M = a_1 A + a_2 Z + a_3 A2/3 + a_4 (A - 2Z) + a_5 Z(Z - 1)2 + a_6 f(A) \ldots\ldots\ldots\ldots (7)$$

Where:

f(A) = 1/A for references 1 and 2.
f(A) = 1/A3/4 for references 3, 4, 5, 6.
f(A) = 1/A1/2 for reference 7.

The Least Numerical Variation Method is a computational physics and chemistry technique used to estimate the basic energy (ground state energy) of quantum systems such as atoms, molecules or nuclides. This method is generally used when analytical solutions are unavailable or impractical. This method is based on the variational principle, where the system energy is estimated by varying the trial wave function used in the calculations. The main goal is to find the test wave function that gives the lowest energy (basic energy).

Numerical approaches are generally used to find the smallest variations. This method involves numerical techniques such as numerical integration, solving partial differential equations, and numerical optimisation to calculate the energy expectation value in the context of quantum mechanics. The advantage of this numerical method is that it can be used for complex quantum systems where analytical calculations are impossible. In addition, this method can be adapted to various situations, including using different basis sets to improve the accuracy of the results.

This method varies the value of *i* from 1 to 6. The variations start with a_1. The initial value taken is the price given by Kaplan. [19]. a1 is varied numerically to obtain the lowest value of the closeness of the experimental results to the calculation results of Equation 8.

$$delta = \sum_{i=1} \left| M_{i(\exp)} - M_{i(\text{model})}) \right| \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (8)$$

The variation of a1 is driven from the initial value $a_{1\omega}$, whose magnitude is a1-nh, where h is the step length, set h = 0.00001 and n taken 1000 times. The lowest delta price is taken by moving $a_{1\omega} = a_{1\omega} + h$ by 2n steps. After the best a1 price is obtained, the same procedure is carried out to find other ai prices. After all the best ai are obtained, the procedure can be repeated using *a* smaller *h* value for the second iteration.

Nuclide stability tests can also be carried out based on the water drop model by looking for the relationship between Z based on the requirement that the differential of the binding energy concerning Z (with A constant) is equal to zero. This will give the second equation given by equation 9.

$$Z = A / \{1.98 + 0.015 A2/3\} \quad (9)$$

For numerical purposes, it is sufficient to carry out numerical variations of Z (fixed A) and take the value of Z that gives the lowest binding energy.

3.0 RESULT AND DISCUSSION

3.1 Delta Comparison of Liquid Drop Model

In Table 1, a comparison of delta is shown as the cumulative deviation price against the experimental price. From the results of this comparison, it can be seen that the numerical variation method provides the smallest deviation with parameter values that are better than the parameters given by several researchers. Meanwhile, the relationship between Z and A for stable nuclides, as required by Segre, is closer to the truth for mass numbers below 20. In this study, the Least Numerical Variation Method gives the smallest delta value of 1.0451118, indicating a powerful approach for calculating the fundamental energy of quantum systems. These results are close to the values predicted from standard theory for similar systems, indicating satisfactory accuracy in modelling the quantum properties of the generated energy. The use of the Least Numerical Variation Method in

ISSN: 2672-7188 e-ISSN: 2682-8820 Vol. 7 No. 1 2025

this research is justified by its ability to adapt to system complexity and flexibility in selecting the appropriate test wave function [20], [21], [22].

Table 1. Comparison of Liquid Drop Model Coefficients

a	Budi *	Segre	Elton	Kaplan	Godfrey	Vincent	Keenan
1	0.9935337	0.9917550	0.9917400	0.9939100	0.9917400	0.9918700	0.9938400
2	- 0.0008502	0.0008400	- 0.0008390	- 0.0008500	- 0.0008390	- 0.0008390	- 0.0008390
3	0.0141000	0.0191100	0.0141000	0.0140000	0.0191150	0.0191270	0.0139614
4	0.0209428	0.1017500	0.0210000	0.8300000	0.1017500	0.0254526	0.0204051
5	0.0006300	0.0007630	0.0006300	0.0006270	0.0007626	0.0007625	0.0006390
6	- 0.0150551	- 0.0130000	- 0.1450000	- 0.0360000	- 0.0360840	- 0.0365140	- 0.0359774
.							
.							
.							
n							
Δ	1.0451118	67.0478400	10.4621600	49.8922900	49.8064600	2.1128820	7.7187860

3.2 Comparison with Other Methods

Table 2 presents an example of a comparison between the various parameters used. The numerical variation method provides calculation results closer to the experimental results. The small deviation or deviation from the experimental values leads to the conclusion that the liquid drop model for calculating the mass of nuclides is quite representative. Thus, estimates of the energy released from a nuclear reaction can be made if the nuclides resulting from the response are known. From Table 2, it can be seen that the proposed research results produce values close to the experimental calculation results. The error value given by the method proposed in this research is 0.00088% or 8.84 $x10^{-6}$.

Nuclide droplets, or specific nuclides, have important applications in medicine, industry, energy, research, and the environment. In medicine, radioactive isotopes such as technetium-99m are used for diagnostic imaging, while iodine-131 aids in thyroid cancer therapy. In industry, nuclides are used for leak detection, radiography, and measuring the thickness of materials. In energy, isotopes such as uranium-235 and plutonium-239 are used as fuel for nuclear reactors, while plutonium-238 is used in radioisotope thermoelectric generators for space missions. Nuclides also play a role in research, such as radiometric dating with carbon-14 and tracking biological reactions. In the environment, isotopes monitor pollution and track water flows. Additionally, nuclides support security through explosives detection and cargo screening. These broad applications demonstrate the importance of nuclides in modern technology.

Table 2. Comparison between various calculations and experiments

Z	A	EXP	PRESENT	SEGRE	ELTON	KAPLAN	GODFREY	VINCENT	KEENAN
68	164	164.930	164.930	165.479	165.000	165.348	165.363	164.941	164.981
67	165	165.930	165.931	166.451	166.001	166.325	166.334	165.942	165.984
68	166	166.932	166.932	167.477	167.002	167.346	167.360	166.943	166.984
68	167	167.932	167.933	168.505	168.005	168.370	168.388	167.945	167.986
68	168	167.934	167.933	168.399	168.004	168.281	168.279	167.945	167.987
70	168	168.934	168.933	169.475	169.005	169.344	169.356	168.945	168.986
69	169	169.936	169.936	170.562	170.009	170.418	170.446	169.949	169.990
68	170	169.935	169.934	170.449	170.007	170.322	170.328	169.947	169.989
70	170	170.936	170.935	171.473	171.007	171.342	171.353	170.947	170.989
70	171	171.936	171.936	172.501	172.010	172.366	172.381	171.949	171.991
70	172	172.938	172.938	173.528	173.011	173.388	173.407	172.950	172.991
70	173	173.939	173.939	174.557	174.013	174.412	174.437	173.953	173.994
70	174	173.940	173.938	174.447	174.013	174.320	174.324	173.952	173.995
72	174	174.941	174.939	175.526	175.013	175.386	175.404	174.952	174.994
71	175	175.943	175.943	176.616	176.018	176.461	176.495	175.957	175.998
70	176	175.942	175.940	176.499	176.015	176.363	176.375	175.954	175.997
72	176	176.943	176.941	177.524	177.016	177.384	177.401	176.954	176.997
72	177	177.944	177.943	178.553	178.019	178.408	178.429	177.957	177.999
72	178	178.946	178.944	179.580	179.020	179.430	179.456	178.958	179.000
72	179	179.947	179.946	180.610	180.022	180.455	180.486	179.961	180.002
72	180	179.947	179.945	180.497	180.021	180.360	180.370	179.960	180.003
74	180	180.948	180.946	181.578	181.022	181.428	181.453	180.960	181.002
73	181	181.948	181.947	182.550	182.024	182.404	182.423	181.962	182.005
74	182	182.950	182.948	183.576	183.025	183.426	183.449	182.963	183.005
74	183	183.951	183.949	184.606	184.028	184.451	184.479	183.965	184.008
74	184	183.953	183.950	184.497	184.028	184.359	184.366	183.966	184.010
76	184	184.953	184.950	185.575	185.028	185.424	185.446	184.965	185.008
75	185	185.954	185.953	186.664	186.032	186.499	186.537	185.969	186.011
74	186	186.956	186.952	187.574	187.031	187.423	187.443	186.968	187.011
76	187	187.956	187.954	188.602	188.034	188.447	188.472	187.971	188.014
76	188	188.958	188.955	189.630	189.035	189.469	189.499	188.971	189.014
76	189	189.959	189.957	190.660	190.038	190.495	190.529	189.974	190.017
76	190	190.961	190.957	191.628	191.038	191.468	191.496	190.974	191.017
77	191	191.961	191.960	192.720	192.042	192.544	192.589	191.978	192.021
76	192	192.963	192.960	193.686	193.042	193.516	193.554	192.978	193.021
77	193	193.963	193.961	194.656	194.044	194.491	194.522	193.980	194.023
78	194	194.965	194.963	195.684	195.045	195.514	195.550	194.981	195.024
78	195	195.965	195.964	196.715	196.048	196.539	196.581	195.984	196.027
78	196	195.966	195.964	196.600	196.048	196.443	196.462	195.984	196.028
80	196	196.967	196.965	197.683	197.049	197.512	197.547	196.984	197.027
79	197	197.968	197.968	198.776	198.053	198.590	198.642	197.988	198.030
78	198	197.967	197.967	198.654	198.051	198.488	198.517	197.986	198.030
80	198	198.968	198.968	199.681	199.052	199.510	188.544	198.987	199.031
80	199	199.968	199.969	200.711	200.055	200.535	200.574	199.990	200.033
80	200	200.970	200.971	201.740	201.056	201.559	201.602	200.991	201.034
80	201	201.971	201.973	202.771	202.059	202.585	202.633	201.994	202.037
80	202	202.972	202.974	203.738	203.059	203.557	203.599	202.994	203.037
81	203	203.974	203.977	204.833	204.064	204.637	204.696	203.998	204.041
80	204	203.973	203.975	204.709	204.062	204.533	204.568	203.997	204.040
82	204	204.974	204.977	205.798	205.064	205.607	205.659	204.998	205.041
81	205	205.974	205.978	206.767	206.066	206.581	206.626	206.000	206.044
82	206	206.976	206.980	207.796	207.067	207.605	207.655	207.001	207.044
82	207	207.977	207.982	208.828	208.070	208.632	208.687	208.004	208.047

ISSN: 2672-7188 e-ISSN: 2682-8820 Vol. 7 No. 1 2025

4.0 CONCLUSION

The small deviation or deviation from the experimental values suggests that the liquid drop model for calculating the mass of nuclides is quite representative. Thus, estimates of the energy released from a nuclear reaction can be made if the nuclides resulting from the response are known. The magnitude of the error delta in the numerical method proposed in this study is 1.00. This value gives an error rate for research results of 0.00088%, equivalent to 8.84×10^{-6}. Suggestions for future research can develop this numerical method for other applications.

ACKNOWLEDGMENTS

Thank you to all parties who have supported the results of this research, especially the Faculty of Engineering and Science, National University.

REFERENCES

[1] A. Abbas, J. M. Islamia, N. Krishna, and N. Akhtar, "Who proposed the liquid drop model of the nucleus first - Gamow or Bohr ?," *ReserachGate*, no. June, pp. 0–8, 2023, doi: 10.13140/RG.2.2.24006.86082.

[2] V. Zelevinsky and A. Volya, "Liquid Drop Model," *Phys. At. Nucl.*, no. February 2017, pp. 91–111, 2017, doi: 10.1002/9783527693610.ch5.

[3] F. Aumayr, K. Ueda, and E. Sokell, "Roadmap on photonic, electronic and atomic collision physics : III. Heavy particles : with zero to relativistic speeds," *J. Phys. B At. Mol. Opt. Phys. ROADMAP*, 2022.

[4] D. Dubbers and M. G. Schmidt, "The neutron and its role in cosmology and particle physics," *Rev. Mod. Phys.*, vol. 83, no. 4, pp. 1–91, 2011, doi: 10.1103/RevModPhys.83.1111.

[5] R. S. oglu Isayev, "Semi-Empirical Formula for Binding Energy on the Basis of Deuteron Clusterization of the Atomic Nucleus," *J. Sci. Educ.*, vol. 53, no. January, pp. 2–6, 2018, doi: 10.20861/2312-8089-2018-53-005.

[6] N. Darmawan and A. N. Zazilah, "Perbandingan Metode Halley dan Olver dalam Penentuan Akar-akar Penyelesaian Polinomial Wilkinson," *J. Teor. dan Apl. Mat.*, vol. 3, no. 2, pp. 93–97, 2019, doi: https://doi.org/10.31764/jtam.v3i2.991.

[7] D. P. Dennis and D. Scherler, "A Combined Cosmogenic Nuclides Approach for Determining the Temperature-Dependence of Erosion," *J. Geophys. Res. Earth Surf.*, vol. 127, no. 4, Apr. 2022, doi: 10.1029/2021JF006580.

[8] J. Eysermans *et al.*, "REGAL International Program: Analysis of experimental

data for depletion code validation," *Ann. Nucl. Energy*, vol. 172, p. 109057, 2022, doi: 10.1016/j.anucene.2022.109057.

[9] S. Qi *et al.*, "Radionuclide identification method for NaI low-count gamma-ray spectra using artificial neural network," *Nucl. Eng. Technol.*, vol. 54, no. 1, pp. 269–274, 2022, doi: 10.1016/j.net.2021.07.025.

[10] G. A. Kovaltsov and I. G. Usoskin, "A new 3D numerical model of cosmogenic nuclide 10Be production in the atmosphere," *Earth Planet. Sci. Lett.*, vol. 291, no. 1–4, pp. 182–188, 2010, doi: 10.1016/j.epsl.2010.01.011.

[11] Q. Wang *et al.*, "Numerical study of the effect of operation parameters on particle segregation in a coal beneficiation fluidized bed by a TFM-DEM hybrid model," *Chem. Eng. Sci.*, vol. 131, pp. 256–270, 2015, doi: 10.1016/j.ces.2015.03.063.

[12] E. Segrè and K. K. Seth, "Experimental Nuclear Physics, Vol. 3," *Phys. Today*, vol. 14, no. 5, p. 50, May 1961, doi: 10.1063/1.3057556.

[13] B. Santoso, "QUANTUM ESTIMATES OF ALPHA EMITTER LIFE TIME Budi Santoso," *Cent. Partnersh. Nucl. Technol. Natl. Nucl. Energy Agency*, pp. 1–9, 2006, doi: ttps://doi.org/10.17146/aij.2006.113.

[14] I. Kaplan, *Nuclear Physics*. in Addison-Wesley series in nuclear science and engineering. Addison-Wesley, 1963. [Online]. Available: https://books.google.co.id/books?id=__pQAAAAMAAJ

[15] S. Godfrey, "Comment on Z′′s and the H1 and ZEUS High Q2 Anomalies," *Mod. Phys. Lett. A*, vol. 12, no. 25, pp. 1859–1863, Aug. 1997, doi: 10.1142/S0217732397001898.

[16] H. Yuan, W. Deng, X. Zhu, G. Liu, and V. S. J. Craig, "Colloidal Systems in Concentrated Electrolyte Solutions Exhibit Re-entrant Long-Range Electrostatic Interactions due to Underscreening," *Langmuir*, vol. 38, no. 19, pp. 6164–6173, May 2022, doi: 10.1021/acs.langmuir.2c00519.

[17] P. Van Duppen, L. Weissman, S. Nuclear, D. Ackermann, and S. Hofmann, "A triplet of differently shaped spin-," *Nature*, no. July 2014, 2000, doi: 10.1038/35013012.

[18] R. S. Harmon, "Atomic Number, Mass Number, and Isotopes BT - Encyclopedia of Geochemistry: A Comprehensive Reference Source on the Chemistry of the Earth," in *White, W.M. (eds) Encyclopedia of Geochemistry. Encyclopedia of Earth Sciences Series.*, W. M. White, Ed., Cham: Springer International Publishing, 2018, pp. 83–85. doi: 10.1007/978-3-319-39312-4_244.

[19] I. Kaplan, *NUCLEAR PHYSICS*. 1977.

[20] A. I. Diveev, "Small Variations of Basic Solution Method for Non-numerical Optimization," *IFAC-PapersOnLine*, vol. 48, no. 25, pp. 28–33, 2015, doi: 10.1016/j.ifacol.2015.11.054.

[21] M. Al-Baali and R. Fletcher, "Variational Methods for Non-Linear Least-

Squares," *J. Oper. Res. Soc.*, vol. 36, no. 5, pp. 405–421, May 1985, doi: 10.1057/jors.1985.68.

[22] S. Mungkasi, "An Accurate Analytical-Numerical Iterative Method for the Susceptible-Infected-Recovered Epidemic Models," *(Jurnal Teor. dan Apl. Mat.*, vol. 5, no. 2, pp. 262–275, 2021, doi: https://doi.org/10.31764/jtam.v5i2.3876 This.