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YOMS v1.0

User Manual and Reproducibility Guide

Yemeni Optical Model System

Optical-Model Calculations for Neutron-Induced Reactions

Verified worked example in this edition: ^{56}Fe

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AUTHOR'S PREFACE

A general guide to the Yemeni Optical Model System

It is my pleasure to present the YOMS v1.0 User Manual and Reproducibility Guide. The Yemeni Optical Model System (YOMS) was developed within the National Atomic Energy Commission as a scientific computational framework for organizing, executing, and documenting optical-model calculations of neutron-induced reactions.

This manual is intentionally a guide to the system as a whole, rather than to a single nuclide. It describes the scientific formulation, computational workflow, required inputs, generated outputs, verification records, interpretation boundaries, and reproducibility practices that govern a YOMS calculation.

Neutron-induced ^{56}Fe is included as the verified worked example in this edition because it currently provides the most complete recorded chain from model parameters and numerical

execution to preserved results and comparison evidence. The use of ^{56}Fe as the worked example in this edition does not limit YOMS to iron. YOMS is designed as a general computational framework for neutron-induced optical-model calculations and may be applied to other nuclides.

I hope this guide provides researchers, reviewers, and institutional users with a clear and citable account of what YOMS does, how its calculations are examined, and where its present evidence boundaries lie. Transparency about both capability and limitation is essential to the responsible development and use of scientific software.

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	dataset, development repository, or third-party software is distributed, and no software licence or redistribution permission is granted

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Abstract

This manual presents the scientific purpose, mathematical formulation, computational organization, and reproducibility principles of the Yemeni Optical Model System (YOMS) v1.0 for optical-model calculations of neutron-induced reactions. To demonstrate the calculation method without implying equal validation for every target, this edition uses neutron-induced 56Fe as its verified worked example and numerical reproducibility record. The example employs a KD2003-form implementation, the YOMS mass-derived Fermi-energy convention, and the native Python solver; that convention differs from the global Fermi-energy expression stored in RIPL OMP record 2405. The guide defines the implemented conventions, records numerical regression criteria, and distinguishes general system capability from target-specific software verification, regression reproduction, numerical agreement, experimental comparison, and scientific interpretation. Evidence for the 56Fe example does not by itself establish validation for other nuclides, exact evaluated-parameter identity with the global record-2405 retrieval, universal physical validity, cross-platform portability, broad reaction-channel validation, or end-to-end regeneration of all preserved comparison products.

Document purpose and status

This document is the institutional public user manual and reproducibility guide for YOMS v1.0. It is intended to let a qualified reader understand, execute, and inspect the documented workflow without turning repository registration, preserved output, or a passing regression test into a stronger scientific claim than the evidence permits.

The document is technically complete as a bounded user manual. The detailed evidence inventories, hashes, coefficient audit, and audit boundaries are placed in appendices so that the operating instructions remain primary. Publication of the manual grants no software licence, repository access, or permission to redistribute YOMS or associated third-party materials.

Version relationship

YOMS v1.0 is the institutional documentation identity for the controlled system described by the author. The current internal Python package metadata reports version 0.1.0. Authorized users should record both identities when preserving a calculation; publication of this manual does not designate or distribute a software archive.

KD2405 is a repository alias associated with Koning–Delaroche 2003 (KD2003) and RIPL OMP record 2405. KD2405 is not a separate physical model. In this snapshot, selecting that alias invokes the YOMS frozen mass-derived Fermi-energy convention; it does not perform an exact numerical retrieval of the global record.

Intended audience

The manual is written for nuclear-reaction researchers, scientific-software reviewers, and reproducibility assessors who can interpret optical-model quantities and who need to:

- understand the general YOMS calculation workflow and run the verified 56Fe worked example from the repository root;
- inspect integrated cross sections and partial-wave S-matrix records;
- reproduce the selected regression behavior;
- compare calculations with preserved experimental-comparison data within stated boundaries; and
- retain adequate environment, command, and file provenance.

Revision history

Revision	Date	Status	Summary
Phase 2	2026-07-13	Internal draft	Evidence-based manual established from the Phase 1 audit.
Phase 3	2026-07-14	Internal draft	Added scientific foundations, authoritative references, professional front matter, clarified terminology, and moved audit detail to appendices.
Phase 3C	2026-07-15	Internal draft	Corrected the spin-operator convention, documented the full $U = -S$ mapping, and distinguished the YOMS mass-derived Fermi energy from the global record-2405 expression.
Phase 3E	2026-07-16	Controlled internal correction	Corrected mass-unit notation, separated repository-wide verification from scientific reproduction, completed metadata placeholders, normalized references, and moved detailed audit evidence to technical appendices.
Phase 3F	2026-07-16	Internal review copy	Recorded the sole-author metadata, affiliation, corresponding-author contact, funding, acknowledgments, and conflict-of-interest statement.
RC1	2026-07-28	Pre-publication review	Prepared and streamlined the institutional manual, added the NATEC-branded cover, clarified the general system scope and the 56Fe worked-example evidence boundary, added the conclusion, external-resource definitions and links, planned NATEC landing page, bounded availability statement, and reviewer-facing citation.
RC2	2026-07-28	Pre-publication review	Added the signed Author's Preface, preserved the system-wide YOMS scope, and clarified that 56Fe is the verified worked example rather than the system boundary.
RC3	2026-07-29	Pre-publication review	Added the institutional back cover and print-wrap cover specification; retained the publication-approval, public-URL, rights, and non-distribution gates.
v1.0	2026-07-29	Final publication master	Authorized by the author for NATEC website publication; removed pre-publication status labels, finalized the citation and public-access wording, and retained the manual-only non-distribution and scientific-evidence boundaries.

Symbols, units, and abbreviations

Symbol or abbreviation	Meaning	Unit or convention
A	Target mass number	dimensionless; $A = 56$ in the worked example
a_i	Diffuseness for potential term i	fm
E_{lab}	Projectile laboratory energy	MeV
E_{cm}	Center-of-mass energy	MeV
EXFOR	Experimental Nuclear Reaction Data Library	database name
$f(r;R,a)$	Woods–Saxon form factor	dimensionless
$g(r;R,a)$	Positive derivative-Woods–Saxon surface form factor	dimensionless
$\hbar c$	Reduced Planck constant times speed of light	MeV fm
j	Total single-particle angular momentum	half-integer
k	Center-of-mass wave number	fm^{-1}
KD2003	Koning–Delaroche global optical model published in 2003	model name
KD2405	Repository alias for KD2003/RIPL OMP record 2405	alias only
ℓ	Orbital angular momentum	non-negative integer
μ	Numerical neutron–target reduced mass	atomic mass units; numerical value used with $m_u c^2$
$m_u c^2$	Atomic-mass energy equivalent used by the solver	931.494013 MeV
OMP	Optical-model potential	abbreviation
RIPL	Reference Input Parameter Library	database name
$S_{\ell j}$	Partial-wave S-matrix element	complex, dimensionless
$T_{\ell j}$	Transmission coefficient $1 - \lvert S_{\ell j} \rvert^2$	dimensionless
U	Signed physical optical potential used in the standard radial equation	MeV
$\mathcal{S}$	Positive-depth complex strength assembled by the repository	MeV
$\xi_{\ell j}$	Dimensionless eigenvalue $\langle \sigma \cdot \mathbf{l} \rangle = \langle 2\mathbf{l} \cdot \mathbf{s} \rangle$	ℓ or $-(\ell+1)$
σ	Integrated cross section	barn in public output

Unless otherwise stated, energies are MeV, distances are fm, and integrated cross sections are barns.

Recommended citation

Recommended citation:

Al-Shami, A. (2026). Yemeni Optical Model System (YOMS) v1.0 User Manual and Reproducibility Guide. National Atomic Energy Commission (NATEC), Aden, Republic of Yemen. Version 1.0. Available at: https://natec-ye.org/yoms/.

When required by a journal, include the date on which the public NATEC record was accessed.

Table of contents

1. Scope and evidence policy

At the system level, YOMS is documented as a framework for optical-model calculations of neutron-induced reactions, including nuclear-system definition, optical-potential evaluation, numerical solution, result handling, and reproducibility controls. The verified scientific evidence in this edition is deliberately narrower: 56Fe is the worked example executed through the recorded Python path using the KD2003 functional form and the YOMS mass-derived Fermi-energy convention described in Section 3.9. Results from that example must not be treated as target-specific validation for another nuclide, projectile, optical potential, or backend. Association with RIPL OMP record 2405 identifies model provenance and coefficient context; it does not assert exact evaluated-parameter identity with the global record retrieval.

The following evidence policy applies:

- source inspection establishes what code is present, not that every path is operational;
- execution establishes behavior only for the command, files, and environment used;
- a passing software test establishes its stated regression condition, not physical validation;
- preserved comparison data can support a bounded experimental comparison but are not described as regenerated end to end unless the complete data pipeline was rerun;
- numerical agreement is a quantified relationship between values and is distinct from scientific interpretation;
- scientific interpretation requires domain review and cannot be inferred from a checksum or test result.

Executed expressions, data records, and tests control the implementation evidence in this manual. Comments or docstrings that use “validated,” mix signed-potential and positive-strength conventions, or describe broader capability are not independent scientific evidence and do not override executed behavior.

2. System identity and maturity terminology

YOMS separates nuclear-system objects, optical-potential evaluation, numerical solution, backend adaptation, data-access utilities, validation artifacts, and reporting. This manual uses the following maturity classes consistently.

Class	Meaning in this manual
Verified	Executed in the recorded environment with stated output and objective acceptance criteria.
Operational but not validated	Executes, but the available evidence does not establish adequate agreement with independent physical reference data.
Experimental	Incomplete, unstable, internally scoped, or not approved as a public production interface.
Placeholder	Registered or represented structurally, but no functioning calculation implementation was verified.
Unavailable	Cannot be used through the documented public workflow.
Host-dependent	Depends on a bundled or external executable, host architecture, operating system, runtime, or environment outside the documented Python calculation.

These labels apply to the specified repository snapshot and evidence boundary, not to the scientific capability of similarly named external programs.

2.1 External codes and nuclear-data resources

The following external programs and nuclear-data resources are identified for scientific context and attribution. Their inclusion in this table does not mean that their software or database files are distributed with YOMS or with this manual.

Resource	Full name and brief description	Role and status in YOMS v1.0	Official resource
ECIS06	Code system for solving coupled differential equations used in optical-model and coupled-channels nuclear-reaction calculations.	External, host-dependent program cited for historical and methodological context; the YOMS public adapter is not documented as operational, and no ECIS06 executable is distributed.	RSICC ECIS-06 record
SCAT2000	Spherical optical-model scattering code used to calculate cross sections, angular distributions, and transmission coefficients.	Placeholder or historical benchmark context only; no functioning public YOMS calculation backend or SCAT2000 executable is distributed.	IAEA RIPL documentation
TALYS	General-purpose nuclear-reaction simulation program covering multiple reaction mechanisms and observables.	Placeholder and historical comparison context only; TALYS is not an operational YOMS v1.0 backend, and its software is not distributed with the manual.	IAEA TALYS
RIPL	Reference Input Parameter Library maintained by the IAEA for nuclear-reaction calculations and nuclear-data evaluation.	Provides model provenance and the global OMP record-2405 comparison context; RIPL database files are not distributed with the public manual.	IAEA RIPL-3
EXFOR	Experimental Nuclear Reaction Data Library coordinated through the international Nuclear Reaction Data Centres network.	Source context for the preserved 56Fe experimental-comparison evidence; the public manual does not distribute the EXFOR database or raw data files.	IAEA EXFOR

3. Scientific foundations and implemented conventions

This chapter states equations only where their relationship to repository code can be identified. The equation-to-source map appears in Section 3.8. References provide the broader scientific context; repository source is the controlling evidence for the conventions actually used here.

3.1 Laboratory-to-center-of-mass kinematics

The native solver forms the numerical reduced mass in atomic-mass units and the center-of-mass energy as

$$\mu = \frac{m_n m_T}{m_n + m_T}, \tag{1}$$

$$E_{cm} = E_{lab}\frac{m_T}{m_n + m_T}, \tag{2}$$

The solver uses the atomic-mass energy equivalent

$$m_u c^2 = 931.494013 \;\; MeV,$$

and forms the wave number as

$$k = \frac{\left(2\mu m_u c^2 E_{cm}\right)^{1/2}}{\hbar c}, \tag{3}$$

where m_n and m_T are the neutron and target masses expressed in atomic mass units, μ is their numerical reduced mass in atomic mass units, and $\hbar c = 197.3269601 \;\; MeV\,fm$. These are the constants and conversions in `modern_omp/solvers/smatrix.py`. Equations (1)–(3) are consistent with standard nonrelativistic optical-model kinematics [1,2].

3.2 Radial Schrödinger equation and repository sign convention

For a neutral projectile and a local partial-wave optical potential, the standard reduced radial equation can be written

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu m_u c^2}{(\hbar c)^2}U_{\ell j}(r,E)\right]u_{\ell j}(r) = 0. \tag{4}$$

The repository potential provider assembles positive well-depth functions into a complex quantity denoted here by $\mathcal{S}_{\ell j}$. The solver adds that strength to its local wave-number function. Its implemented convention is therefore represented by

$$U_{\ell j}(r,E) = -\mathcal{S}_{\ell j}(r,E), \tag{5}$$

and

$$q_{\ell j}(r) = k^2 - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu m_u c^2}{(\hbar c)^2}\mathcal{S}_{\ell j}(r,E), \tag{6}$$

with $u''_{\ell j} + q_{\ell j} u_{\ell j} = 0$. Equations (3), (4), and (6) now use $m_u c^2$ rather than the ambiguous symbol u, so the atomic-mass conversion is explicit and does not collide with the radial function $u_{\ell j}$. This is a manual correction: the solver already contains the conversion through its CK2 constant. Equation (6) is evaluated by q_at in modern_omp/solvers/smatrix.py and by the frozen reference solver in tools/calculate_fe56_koning_delaroche.py. The mass and sign convention remains subject to qualified review. The complex radial equation is integrated with the repository's Numerov recurrence. The repository is the evidence for that recurrence; no separate numerical-method source has yet been verified against the exact implemented recurrence.

Dimensionally, Equation (3) returns fm^{-1}, while k^2, $\ell(\ell+1)/r^2$, and $2\mu m_u c^2 U/(\hbar c)^2$ in Equation (4), or the corresponding S term in Equation (6), each has unit fm^{-2}.

For the verified 56Fe path, tools/calculate_fe56_koning_delaroche.py sets the matching radius to 1.5 times the largest central-potential radius candidate, uses 700 radial steps, and sets $h = r_{match}/700$. The Python backend delegates this scoped workflow to that frozen solver. These are regression-preserved settings, not a demonstrated convergence result.

3.3 Woods–Saxon form factors

The central form factor implemented in modern_omp/potentials/woods_saxon.py is

$$f(r;R,a) = \frac{1}{1+\exp[(r-R)/a]}. \tag{7}$$

The implemented positive surface form factor is

$$g(r;R,a) = \frac{4\exp[(r-R)/a]}{\left(1+\exp[(r-R)/a]\right)^2} = 4f(1-f). \tag{8}$$

Consequently,

$$\frac{df}{dr} = -\frac{1}{a} f(1-f), g = -4a\frac{df}{dr}. \tag{9}$$

For each geometry term, the provider uses

$$R_i = r_i A^{1/3}, A = 56. \tag{10}$$

Equations (7)–(10) are implemented by woods_saxon and derivative_shape in tools/calculate_fe56_koning_delaroche.py for the verified 56Fe path. The corresponding shapes are represented in modern_omp/potentials/woods_saxon.py and modern_omp/potentials/koning_delaroche.py. The Woods–Saxon form originates with Woods and Saxon [3]; the parameterization and RIPL representation used here are documented by Koning and Delaroche [4] and RIPL [5].

3.4 Complex potential decomposition

For clarity, the repository's positive-depth complex strength can be grouped as

$$\mathcal{S}_{\ell j} = V_v f_v + V_{so} h_{so} \xi_{\ell j} + i\left(W_v f_w + W_d g_d + W_{so} h_{so} \xi_{\ell j}\right), \tag{11}$$

where the implemented spin–orbit radial factor is

$$h_{so}(r) = \lambda_\pi^2 \frac{\exp[(r-R_{so})/a_{so}]}{a_{so} r\left(1+\exp[(r-R_{so})/a_{so}]\right)^2} = -\lambda_\pi^2 \frac{1}{r}\frac{df_{so}}{dr}, \tag{12}$$

and

$$\lambda_{\pi}^{2}=\left(\frac{\hbar c}{\left(m_{\pi^{0}}+2m_{\pi^{\pm}}\right)/3}\right)^{2}. \tag{13}$$

In the implemented convention, $m_{\pi^{0}}=134.9645\ MeV$ and $m_{\pi^{\pm}}=139.5688\ MeV$, with masses represented in energy units. These repository constants reproduce $\lambda_{\pi}^{2}=2.043621648203108\ fm^{2}$. This is implementation documentation, not a new physical determination.

The solver supplies the dimensionless spin–orbit eigenvalue

$$\xi_{\ell j}\equiv\langle\sigma\cdot\boldsymbol{l}\rangle=\langle 2\,\boldsymbol{l}\cdot\boldsymbol{s}\rangle,$$

where $\sigma=2\mathbf{s}$ for the spin-one-half neutron. The implemented variable is therefore the eigenvalue of $\sigma\cdot\mathbf{l}$, not the eigenvalue of unscaled $\mathbf{l}\cdot\mathbf{s}$. Its branch values are

$$\xi_{\ell j}=\begin{cases}\ell, & j=\ell+\dfrac{1}{2},\\ -(\ell+1), & j=\ell-\dfrac{1}{2}.\end{cases} \tag{14}$$

Thus Equation (11) contains the real central, imaginary volume, imaginary surface, and complex spin–orbit terms actually assembled by the executed functions in the frozen 56Fe solver and package provider. The implementation stores positive-depth terms in $S_{\ell j}$; Equation (5) transforms the complete stored strength into the signed potential $U_{\ell j}=-S_{\ell j}$ used in the conventional radial equation. The Phase 3B convention audit found the derivative Woods–Saxon signs, absorptive-term signs, $\sigma\cdot\boldsymbol{l}$ normalization, and pion-length factor consistent with the inspected KD2003/RIPL conventions after applying this explicit mapping.

The docstring attached to the frozen optical_strengths function is not authoritative scientific evidence: it mixes signed-potential and positive-strength conventions and labels the spin operator imprecisely. This is a documentation defect. The audit did not find a corresponding solver-sign defect.

3.5 External-wave matching and S-matrix convention

For the neutral-particle asymptotic match, the solver evaluates Riccati–Bessel functions

$$F_{\ell}(\rho)=\rho\,j_{\ell}(\rho),G_{\ell}(\rho)=-\rho\,y_{\ell}(\rho),\rho=k\,r. \tag{15}$$

Using the numerical solution u and radial derivatives at the matching radius, the implemented matching ratio is

$$K_{\ell j}=\frac{u\,F_{\ell}^{'}-u^{'}F_{\ell}}{u^{'}G_{\ell}-u\,G_{\ell}^{'}}, \tag{16}$$

Here $K_{\ell j}$ is the dimensionless matching ratio generated by the stated neutral-function convention at the matching radius.

followed by

$$S_{\ell j}=\frac{1+i\,K_{\ell j}}{1-i\,K_{\ell j}}. \tag{17}$$

The repository reports the transmission coefficient as

$$T_{\ell j}=1-|S_{\ell j}|^{2}. \tag{18}$$

Equations (15)–(18) map directly to spherical_fg and s_matrix in tools/calculate_fe56_koning_delaroche.py for the verified path. The general solver represents these conventions in spherical_fg, neutron_s_matrix, and SMatrixElement in modern_omp/solvers/smatrix.py. Standard S-matrix context is given by Satchler [1] and Newton [2].

3.6 Partial-wave weights and integrated cross sections

The repository stores two spin branches when $\ell > 0$:

$$w_{\ell,+} = \ell + 1 \text{ for } j = \ell + \frac{1}{2}, w_{\ell,-} = \ell \text{ for } j = \ell - \frac{1}{2}. \tag{19}$$

For the verified path, modern_omp/backends/python_solver.py uses $\rho_{est} = (16.0 \ \ fm)k$ and

$$\ell_{max} = max\left(18, \lfloor 2.5\rho_{est}^{0.8} + 12 \rfloor\right).$$

This is the frozen partial-wave cutoff convention. The repository does not establish it as a universal convergence criterion.

The integrated elastic and reaction cross sections are

$$\sigma_{el} = \frac{\pi}{k^2} \sum_{\ell,j} w_{\ell j} |1 - S_{\ell j}|^2, \tag{20}$$

$$\sigma_R = \frac{\pi}{k^2} \sum_{\ell,j} w_{\ell j} \left(1 - |S_{\ell j}|^2\right). \tag{21}$$

The public result defines total integrated cross section by the closure relation

$$\sigma_{tot} = \sigma_{el} + \sigma_R. \tag{22}$$

With the same convention, this is equivalently

$$\sigma_{tot} = \frac{2\pi}{k^2} \sum_{\ell,j} w_{\ell j} \left(1 - \mathrm{Re}\, S_{\ell j}\right). \tag{23}$$

Equation (23) is an algebraic consequence of Equations (20)–(22); it is not separately evaluated by the public cross-section routine. Equation (19) and the cutoff convention map to _frozen_fe56_smatrix in modern_omp/backends/python_solver.py and to elastic_cross_section_b in tools/calculate_fe56_koning_delaroche.py. Equations (20)–(22) map to modern_omp/solvers/cross_sections.py, which integrates the S-matrix rows returned by the verified path. These partial-wave formulas are standard optical-model relations [1,2].

The solver first obtains areas in fm² and returns barns using

$$1 \ \ b = 100 \ \ fm^2. \tag{24}$$

3.7 What these equations do and do not establish

The source mapping establishes the implemented mathematical convention. It does not by itself establish that the parameter convention exactly reproduces an external reference implementation, that every numerical setting is converged, or that the calculation is physically adequate over an unrestricted energy range. Those are separate numerical and scientific questions.

3.8 Equation-to-implementation and reference map

Equations	Subject	Repository implementation evidence	Scientific reference
(1)–(3)	Reduced mass, frame conversion, wave number	tools/calculate_fe56_koning_delaroche.py: constants and s_matrix; modern_omp/solvers/smatrix.py: _kinematics	[1], [2]
(4)–(6)	Radial equation and sign convention	modern_omp/solvers/smatrix.py: neutron_s_matrix, q_at; tools/calculate_fe56_koning_delaroche.py: s_matrix, q_at	[1], [2]; implementation details are repository-defined
(7)–(10)	Woods–Saxon and surface form factors; radii	tools/calculate_fe56_koning_delaroche.py: woods_saxon, derivative_shape, optical_strengths; package forms in modern_omp/potentials/woods_saxon.py	[3], [4], [5]
(11)–(14)	Complex potential and spin–orbit terms	Executed optical_strengths and kd2405_strength bodies plus solver-supplied branch eigenvalues; the frozen docstring is excluded as authoritative evidence	[4], [5]; RIPL Handbook Eqs. (5.1)–(5.2)
(15)–(18)	Neutral matching, S matrix, transmission	tools/calculate_fe56_koning_delaroche.py: spherical_fg, s_matrix; modern_omp/solvers/smatrix.py: spherical_fg, neutron_s_matrix	[1], [2]
(19)–(24)	Cutoff, spin weights, integrated cross sections, closure, units	modern_omp/backends/python_solver.py: _frozen_fe56_smatrix; modern_omp/solvers/cross_sections.py; frozen elastic_cross_section_b	[1], [2]

3.9 KD2003 Optical-Potential Equations and Parameter Tables

This section is the complete parameter reference for the verified worked example: neutron-induced 56Fe calculations with a KD2003-form implementation using the YOMS mass-derived Fermi-energy convention. KD2405 is a repository alias associated with RIPL OMP record 2405; it is not a separate optical-potential model. Because the YOMS Fermi-energy convention differs from the global record expression, the evaluated YOMS depths are not an exact numerical retrieval of the global record. The tables in this section do not describe the preserved historical ECIS-derived outputs.

3.9.1 Published, RIPL-record, and YOMS conventions

Convention level	Meaning in this manual	Evidentiary boundary
Published KD2003 convention	The optical model and parameterization reported by Koning and Delaroche [4].	The publication is the scientific reference. This manual does not independently certify that every repository sign and normalization choice is identical to every notation used in the paper.
RIPL-record convention	Global KD2003 coefficients and the global Fermi-energy expression are stored in RIPL OMP record 2405.	Repository evidence includes resources/RIPL3/optical/om-get/om-parameter-u.dat and resources/RIPL3/optical/om-get/om_retrieve.f; the official IAEA RIPL optical-model distribution is the external authority.
YOMS implementation convention	The package delegates the scoped 56Fe parameters to the frozen evaluator, uses the KD2003 functional form with mass-derived $E_F = -9.4218\ MeV$, constructs a positive-depth strength $S_{\ell j}$, and adds it in the local wave-number function. Relative to Equation (4), $U_{\ell j} = -S_{\ell j}$.	This accurately describes the executed code and preserved baseline. It is not exact evaluated-parameter identity with the global record-2405 retrieval, which gives $E_F = -9.79964\ MeV$ for $A = 56$.

The potential-form convention is resolved narrowly: after the explicit $U=-S$ transformation, the audited derivative Woods–Saxon signs, absorptive signs, spin–orbit normalization, and pion-length factor agree with the inspected KD2003/RIPL conventions. This finding does not resolve the scientific justification for choosing the YOMS mass-derived Fermi energy.

3.9.2 Complete implemented potential

The Woods–Saxon volume form factor f, positive derivative-surface form g, full-radius relation, and spin–orbit eigenvalue are defined in Equations (7)–(10) and (14). In the equations below, r is the radial coordinate in fm, $E=E_{lab}$ is the incident-neutron laboratory energy in MeV, R_i is a full radius in fm, and a_i is a diffuseness in fm. The real central component, with depth $V(E)$ in MeV, is

$$U_V(r,E)=-V(E)f(r;R_V,a_V), \tag{25}$$

With $i=(-1)^{1/2}$ and imaginary-volume depth $W_V(E)$ in MeV, the imaginary volume component is

$$U_{WV}(r,E)=-iW_V(E)f(r;R_{WV},a_{WV}), \tag{26}$$

With derivative-surface depth $W_D(E)$ in MeV and positive surface form g from Equation (8), the imaginary surface component is

$$U_{WD}(r,E)=-iW_D(E)g(r;R_{WD},a_{WD}), \tag{27}$$

The spin–orbit derivative factor is

$$d(r;R,a)=\frac{\exp[(r-R)/a]}{ar\left(1+\exp[(r-R)/a]\right)^2}=-\frac{1}{r}\frac{df(r;R,a)}{dr}, \tag{28}$$

where d has unit fm^{-2}. With $\lambda_\pi^2=2.04362164820311\ \ fm^2$ from Equation (13), spin–orbit eigenvalue $\xi_{\ell j}$ from Equation (14), and real spin–orbit depth $V_{SO}(E)$ in MeV, the real spin–orbit component is

$$U_{VSO,\ell j}(r,E)=-\lambda_\pi^2 V_{SO}(E)d(r;R_{VSO},a_{VSO})\xi_{\ell j}, \tag{29}$$

With signed imaginary spin–orbit depth $W_{SO}(E)$ in MeV, the imaginary spin–orbit component is

$$U_{WSO,\ell j}(r,E)=-i\lambda_\pi^2 W_{SO}(E)d(r;R_{WSO},a_{WSO})\xi_{\ell j}. \tag{30}$$

The complete signed potential used to interpret the radial equation is

$$\begin{aligned}U_{\ell j}(r,E)&=U_V+U_{WV}+U_{WD}+U_{VSO,\ell j}+U_{WSO,\ell j}\\&=-S_{\ell j}(r,E).\end{aligned} \tag{31}$$

The repository functions optical_strengths and kd2405_strength return $S_{\ell j}$, not $U_{\ell j}$. In particular, the implemented W_{SO} values are negative at the reference energies. Equations (29), (30), and (31) preserve that signed coefficient exactly; they do not replace it by its magnitude.

For completeness, the associated form, kinematic, scattering, and observable equations are:

Required relation	Equation
Woods–Saxon form factor f	(7)
Positive derivative Woods–Saxon form $g=4f(1-f)=-4a\,df/dr$	(8), (9)
Full radius $R_i=r_iA^{1/3}$	(10)
Laboratory-to-center-of-mass conversion	(2)

Required relation	Equation
Wave number	(3)
Real central volume term	(25)
Imaginary volume term	(26)
Imaginary derivative-surface term	(27)
Spin–orbit derivative factor	(28)
Real spin–orbit term	(29)
Imaginary spin–orbit term	(30)
Total complex potential	(31)
S matrix and its matching ratio	(16), (17)
Transmission coefficient	(18)
Elastic, reaction, and total integrated cross sections	(20)–(23)
Cross-section unit conversion	(24)

3.9.3 Energy and geometry parameterization

The frozen implementation first calculates the neutron Fermi energy from mass excesses and then forms the shifted energy

$$E_F = round_4\left[-\frac{1}{2}\left(\Delta M_{55} - \Delta M_{57} + 2\,\Delta M_n\right)\right] = -9.4218 \;\; MeV,$$
$$\varepsilon = E_{lab} - E_F. \tag{32}$$

Here $\Delta M_{55} = -57.475472 \;\; MeV$, $\Delta M_{57} = -60.176197 \;\; MeV$, and $\Delta M_n = 8.071388 \;\; MeV$ are the exact constants in tools/calculate_fe56_koning_delaroche.py. The round-to-four-decimal operation is part of the implementation. For the three reference energies, ε equals 10.2218, 10.4218, and 11.4218 MeV.

This is the **YOMS frozen mass-derived convention**. The global KD2003/RIPL record-2405 expression is instead

$$E_F^{global\ RIPL} = -11.2814 + 0.02646\,A,$$

which gives

$$E_F^{global\ RIPL} = -9.79964 \;\; MeV \text{ for } A = 56.$$

The global expression is evidenced by KD2003 Table 10 and by resources/RIPL3/optical/om-get/om-parameter-u.dat; om_retrieve.f applies stored record coefficients when present. The two Fermi energies differ by $0.37784 \;\; MeV$. Because the shifted energy $\varepsilon = E_{lab} - E_F$ enters Equations (33), (36), (38), (41), and (43), the difference changes every energy-dependent optical-potential depth: V, W_V, W_D, V_{SO}, and W_{SO}. It does not change the energy-independent geometry formulas.

The real volume depth is

$$V(\varepsilon) = V_0\left(1 - v_1\varepsilon + v_2\varepsilon^2 - v_3\varepsilon^3\right),$$
$$V_0 = 59.3 - 0.024\,A - 21\,\eta,$$
$$v_1 = 0.007228 - 1.48 \times 10^{-6}\,A,$$

$$v_2 = 1.994 \times 10^{-5} - 2.0 \times 10^{-8} A,$$
$$v_3 = 7.0 \times 10^{-9}. \quad (33)$$

The real-volume reduced radius and diffuseness are

$$r_V = 1.3039 - 0.4054\, A^{-1/3}, \quad (34)$$

$$a_V = 0.6778 - 1.487 \times 10^{-4} A. \quad (35)$$

The imaginary-volume depth is

$$W_V(\varepsilon) = A_V \frac{\varepsilon^2}{\varepsilon^2 + B_V^2},$$
$$A_V = 12.195 + 0.0167\, A,$$
$$B_V = 73.55 + 0.0795\, A, \quad (36)$$

with shared geometry

$$r_{WV} = r_V, a_{WV} = a_V. \quad (37)$$

The derivative-surface depth is

$$W_D(\varepsilon) = A_D e^{-C_D \varepsilon} \frac{\varepsilon^2}{\varepsilon^2 + B_D^2},$$
$$A_D = 16 - 16\eta,$$
$$C_D = 0.018 + \frac{0.003802}{1 + \exp[(A - 156)/8]},$$
$$B_D = 11.5, \quad (38)$$

with geometry

$$r_{WD} = 1.3424 - 0.01585\, A^{1/3}, \quad (39)$$

$$a_{WD} = 0.5446 - 1.656 \times 10^{-4} A. \quad (40)$$

The real spin–orbit depth is

$$V_{SO}(\varepsilon) = (5.922 + 0.003\, A) e^{-0.004\varepsilon}, \quad (41)$$

with geometry

$$r_{VSO} = 1.1854 - 0.647\, A^{-1/3}, a_{VSO} = 0.59 \ \ fm. \quad (42)$$

The imaginary spin–orbit depth is

$$W_{SO}(\varepsilon) = -3.1 \frac{\varepsilon^2}{\varepsilon^2 + 160^2}, \quad (43)$$

with shared spin–orbit geometry

$$r_{WSO} = r_{VSO}, a_{WSO} = a_{VSO}. \quad (44)$$

In Equations (33)–(44), $A = 56$, $Z = 26$, $N = 30$, and $\eta = (N - Z)/A = 1/14$. Depth coefficients and ε are in MeV; v_1, v_2, and v_3 have units MeV^{-1}, MeV^{-2}, and MeV^{-3}, respectively; C_D and 0.004 have units MeV^{-1}; reduced radii and diffusenesses are in fm. Constants such as 156 and 8 in the mass-number logistic term are dimensionless mass-number scales.

Implemented energy-dependence coefficients for 56Fe

Quantity	Implemented expression	Evaluated value	Unit	Sign or role
A, Z, N	fixed scoped nucleus	56, 26, 30	dimensionless	Defines the only nucleus covered here.
η	$(N-Z)/A$	0.0714285714285714	dimensionless	Enters V_0 and A_D.
$A^{1/3}$	$56^{1/3}$	3.82586236554478	dimensionless	Converts reduced radii to full radii.
E_F^{YOMS}	Equation (32), rounded to four decimals	-9.4218	MeV	Frozen mass-derived convention; $\varepsilon = E_{lab} + 9.4218\ \ MeV$.
$E_F^{global\ RI}$	$-11.2814 + 0.026$	-9.79964	MeV	Global record-2405 expression shown for comparison; not used by the frozen YOMS path.
V_0	$59.3 - 0.024A - 2$	56.456	MeV	Positive depth coefficient in S; physical central term is negative in Equation (25).
v_1	$0.007228 - 1.48 \times$	0.00714512	MeV^{-1}	Appears with a minus sign.
v_2	$1.994 \times 10^{-5} - 2.0$	1.882×10^{-5}	MeV^{-2}	Appears with a plus sign.
v_3	7.0×10^{-9}	7.0×10^{-9}	MeV^{-3}	Appears with a minus sign.
$r_V = r_{WV}$	Equation (34)	1.19793696179691	fm	Reduced radius; energy-independent here.
$a_V = a_{WV}$	Equation (35)	0.6694728	fm	Diffuseness; energy-independent here.
A_V	$12.195 + 0.0167A$	13.1302	MeV	Positive numerator coefficient for W_V.
B_V	$73.55 + 0.0795A$	78.002	MeV	Positive scale in the W_V denominator.
A_D	$16 - 16\eta$	14.8571428571429	MeV	Positive surface-depth coefficient.
C_D	Equation (38)	0.0218019858313174	MeV^{-1}	Positive exponential damping coefficient.
B_D	fixed	11.5	MeV	Positive scale in the W_D denominator.
r_{WD}	Equation (39)	1.28176008150612	fm	Reduced surface radius.
a_{WD}	Equation (40)	0.5353264	fm	Surface diffuseness.
$V_{SO,0}$	$5.922 + 0.003A$	6.09	MeV	Positive real spin–orbit coefficient.
λ_{SO}	fixed exponent coefficient	0.004	MeV^{-1}	$V_{SO} = V_{SO,0} e^{-\lambda_{SO}\varepsilon}$.
$r_{VSO} = r_W$	Equation (42)	1.01628780040108	fm	Reduced spin–orbit radius.
$a_{VSO} = a_W$	fixed	0.59	fm	Spin–orbit diffuseness.
A_{WSO}	fixed numerator coefficient	-3.1	MeV	Negative in the implemented W_{SO}.
B_{WSO}	fixed denominator scale	160	MeV	Positive denominator scale.

These values and formulas reproduce the implemented 56Fe evaluator only. They are not a declaration of a supported parameterization beyond the stated scope. A literal-coefficient unit audit is preserved in Appendix E.1.

3.9.4 Master parameter-definition table

Parameter	Physical meaning	Potential component	Unit	Mathematical role	Equation	Exact implementation field or function	Evidence source
V	Real central depth	U_V	MeV	Multiplies f_V with physical sign $-V f_V$	(25), (33)	KDParameters.v; kd_parameters; kd2405_parameters	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column V
r_V	Real central reduced radius	U_V	fm	Gives $R_V = r_V A^{1/3}$	(10), (34)	KDParameters.rv	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column rv
a_V	Real central diffuseness	U_V	fm	Controls the radial falloff of f_V	(7), (35)	KDParameters.av	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column av
W_V	Imaginary volume depth	U_{WV}	MeV	Multiplies f_{WV} with physical factor $-i$	(26), (36)	KDParameters.wv	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column Wv
r_{WV}	Imaginary-volume reduced radius	U_{WV}	fm	Gives $R_{WV} = r_{WV} A^{1/3}$	(10), (37)	KDParameters.rwv	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column rw
a_{WV}	Imaginary-volume diffuseness	U_{WV}	fm	Controls f_{WV}	(7), (37)	KDParameters.awv	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column aw
W_D	Imaginary derivative-surface depth	U_{WD}	MeV	Multiplies positive surface shape g_{WD} with physical factor $-i$	(27), (38)	KDParameters.wd	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column Wd
r_{WD}	Surface reduced radius	U_{WD}	fm	Gives $R_{WD} = r_{WD} A^{1/3}$	(10), (39)	KDParameters.rwd	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column rd
a_{WD}	Surface diffuseness	U_{WD}	fm	Controls g_{WD}	(8), (40)	KDParameters.awd	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column ad
V_{SO}	Real spin–orbit depth	U_{VSO}	MeV	Multiplies $\lambda_\pi^2 d_{VSO} \xi_{\ell j}$	(29), (41)	KDParameters.vso; optical_strengths; kd2405_strength	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column Vso
r_{VSO}	Real spin–orbit reduced radius	U_{VSO}	fm	Gives $R_{VSO} = r_{VSO} A^{1/3}$	(10), (42)	KDParameters.rvso	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column rso
a_{VSO}	Real spin–orbit diffuseness	U_{VSO}	fm	Controls d_{VSO}	(28), (42)	KDParameters.avso	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column aso
W_{SO}	Imaginary spin–orbit signed depth	U_{WSO}	MeV	Multiplies $\lambda_\pi^2 d_{WSO} \xi_{\ell j}$ with factor $-i$; evaluated value is negative	(30), (43)	KDParameters.wso; optical_strengths; kd2405_strength	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; Stage 1 column Wso
r_{WSO}	Imaginary spin–orbit reduced radius	U_{WSO}	fm	Gives $R_{WSO} = r_{WSO} A^{1/3}$	(10), (44)	KDParameters.rwso	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; shared Stage 1 column rso
a_{WSO}	Imaginary spin–orbit diffuseness	U_{WSO}	fm	Controls d_{WSO}	(28), (44)	KDParameters.awso	tools/calculate_fe56_koning_delaroche.py; modern_omp/potentials/koning_delaroche.py; shared Stage 1 column aso

3.9.5 YOMS frozen-implementation parameters using the mass-derived $E_F = -9.4218\ MeV$ convention

The following table was generated by executing `modern_omp.potentials.koning_delaroche.kd2405_parameters` for `Nucleus(26, 56, "Fe")` with the default `preserve_fe56=True` path. That path delegates to the frozen YOMS evaluator. Values are printed with 12 digits after conversion to scientific notation and must not be relabeled as values from an exact global record-2405 retrieval.

The displayed digits are retained for regression traceability. They do not express experimental precision, physical accuracy, or uncertainty.

Parameter	Unit	0.8 MeV	1.0 MeV	2.0 MeV
V	MeV	$5.244327392807 \times 10^{1}$	$5.236695845912 \times 10^{1}$	$5.198664091026 \times 10^{1}$
r_V	fm	1.197936961797	1.197936961797	1.197936961797
a_V	fm	0.669472800000	0.669472800000	0.669472800000
W_V	MeV	0.2216765982748	0.2302824946531	0.2756229754460
r_{WV}	fm	1.197936961797	1.197936961797	1.197936961797
a_{WV}	fm	0.669472800000	0.669472800000	0.669472800000
W_D	MeV	5.247377371666	5.337899585004	5.751548623585
r_{WD}	fm	1.281760081506	1.281760081506	1.281760081506
a_{WD}	fm	0.535326400000	0.535326400000	0.535326400000
V_{SO}	MeV	5.846018795112	5.841343850303	5.818025143407
r_{VSO}	fm	1.016287800401	1.016287800401	1.016287800401
a_{VSO}	fm	0.590000000000	0.590000000000	0.590000000000
W_{SO}	MeV	-0.01260107342294	-0.01309689967550	-0.01571749344156
r_{WSO}	fm	1.016287800401	1.016287800401	1.016287800401
a_{WSO}	fm	0.590000000000	0.590000000000	0.590000000000

Energy-dependent depth comparison: YOMS convention versus global record expression

The comparison below was generated programmatically, not interpolated or manually estimated. The YOMS column was obtained by executing the frozen `kd_parameters` function. The global-record column was obtained by substituting $E_F = -11.2814 + 0.02646\,A = -9.79964\ \ MeV$ into Equations (33), (36), (38), (41), and (43) with the coefficients printed in Section 3.9.3. The absolute difference is $\left|X_{YOMS} - X_{global\ RIPL}\right|$. The relative difference is that absolute difference divided by $\left|X_{global\ RIPL}\right|$; all listed comparison values are nonzero, so the percentage is defined. These percentages quantify convention-dependent numerical differences, not uncertainty.

E_{lab} (MeV)	Depth	YOMS mass-derived value (MeV)	Global-record-expression value (MeV)	Absolute difference (MeV)	Relative difference
0.8	V	52.4432739281	52.2991693093	0.144104618727	0.275539020%
0.8	W_V	0.221676598275	0.238065025863	0.0163884275882	6.88401311%
0.8	W_D	5.24737737167	5.41619598197	0.168818610301	3.11692211%
0.8	V_{SO}	5.84601879511	5.83719002955	0.00882876556406	0.151250268%
0.8	W_{SO}	-0.0126010734229	-0.0135457206021	0.000944647179177	6.97376837%
1.0	V	52.3669584591	52.2230125393	0.143945919781	0.275636952%
1.0	W_V	0.230282494653	0.246963103187	0.0166806085336	6.75429176%
1.0	W_D	5.33789958500	5.50178708057	0.163887495564	2.97880476%
1.0	V_{SO}	5.84134385030	5.83252214493	0.00882170537606	0.151250268%
1.0	W_{SO}	-0.0130968996755	-0.0140593796128	0.000962479937301	6.84582082%
2.0	V	51.9866409103	51.8434879477	0.143152962603	0.276125254%
2.0	W_V	0.275622975446	0.293745435078	0.0181224596320	6.16944383%
2.0	W_D	5.75154862358	5.89125588830	0.139707264713	2.37143433%
2.0	V_{SO}	5.81802514341	5.80923865437	0.00878648903419	0.151250268%
2.0	W_{SO}	-0.0157174934416	-0.0167688636210	0.00105137017943	6.26977596%

The 0.8 MeV global-record-expression values reproduce the Phase 3B audit checkpoint. The 1.0 and 2.0 MeV values were generated with Equations (33), (36), (38), (41), and (43) and the coefficient set printed in Section 3.9.3. The comparison establishes a numerical consequence of the Fermi-energy choice; it does not decide which convention is physically preferable. The percentages are numerical differences between conventions, not uncertainties.

The geometry is energy-independent at these energies in the implemented 56Fe evaluator. Reduced radii r_i and full radii R_i are distinct:

Geometry	Reduced radius r_i (fm)	Full radius $R_i = r_i 56^{1/3}$ (fm)
Real central V	1.197936961797	4.583141938434
Imaginary volume $W V$	1.197936961797	4.583141938434
Imaginary surface $W D$	1.281760081506	4.903837657492
Real spin–orbit $V SO$	1.016287800401	3.888177248117
Imaginary spin–orbit $W SO$	1.016287800401	3.888177248117

The detailed convention cross-check log and complete equation-to-code inventory are preserved in Appendices E.2 and E.3.

4. Verification, reproduction, comparison, and interpretation

4.1 Required distinctions

Evidence category	Question answered	What it does not establish
Software verification	Did a specified command or test behave as expected?	Physical validity
Regression reproduction	Did current output reproduce a preserved numerical baseline within a stated tolerance?	Agreement with experiment or numerical convergence
Numerical agreement	How close are two numerical values under a declared metric?	Causation or scientific adequacy
Experimental comparison	How do calculations compare with experimental records or preserved comparison data?	A universal validation conclusion
Scientific interpretation	What physical explanation or domain conclusion is justified?	This requires qualified judgment beyond software execution

4.2 Verified regression tolerance

The selected regression test compares three integrated cross sections at 0.8 MeV with an absolute delta of

$$5 \times 10^{-11} \ b.$$

This is a **verified regression tolerance**. It is not an experimental uncertainty, parameter uncertainty, convergence certificate, or physical-accuracy threshold.

4.3 Matching language

Where preserved calculated and experimental rows are joined directly, they are described as:

> matched at the same energy or angle without interpolation.

This matching rule does not mean exact numerical agreement between calculation and experiment. It describes only how coordinate values were paired.

4.4 Interpretation of the preserved YOMS baseline

The YOMS frozen 56Fe workflow reproduces its preserved numerical baseline internally. It uses the KD2003 functional form with a YOMS mass-derived Fermi-energy convention. Therefore, internal regression reproducibility must not be interpreted as exact evaluated-parameter identity with the global RIPL record 2405 retrieval.

For the associated paper and any derivative scientific communication:

- identify $E_F = -9.4218 \ \ MeV$ explicitly as the YOMS frozen mass-derived convention;
- do not describe preserved YOMS depths or cross sections as an exact numerical retrieval of global RIPL record 2405;
- keep software verification, regression reproduction, numerical agreement, experimental comparison, and scientific interpretation separate; and
- do not infer physical superiority, universal validation, or an uncertainty statement from internal regression reproduction.

5. Worked example: 56Fe reproduction procedure

5.1 Record provenance

Before calculation, record:

```
pwd
git rev-parse HEAD
git status --short
python3 --version
python3 -c "import platform; print(platform.platform(), platform.machine())"
python3 -c 'import modern_omp; print(modern_omp.__version__)'
```

A nonempty git status is not automatically a failure, but it means the commit identifier alone is insufficient provenance. Record the diff or otherwise preserve the exact modified files.

5.2 Verify selected protected assets

```
python3 tools/verify_frozen_core.py
```

Acceptance criterion: exit status zero and the message:

```
Frozen core verification: PASS (430 files)
```

The verifier covers the selected frozen-core manifest, not the entire repository.

5.3 Execute the reference calculation

```
python3 examples/fe56.py
python3 examples/fe56_elastic.py
```

Acceptance criteria are the numerical values in Appendix A, subject to the verified regression tolerance only where that tolerance is actually asserted by the relevant test.

5.4 Archive the calculation record

Preserve the following reproducibility record in accordance with general computational-research and data-stewardship principles [10,11]:

- repository commit and dirty-tree status;
- environment and dependency versions;
- exact commands;
- console output and exit status;
- the relevant hashes in Appendix A;
- captured or user-serialized calculation output, if produced; and
- any differences from the recorded environment.

6. Preserved experimental-comparison evidence

The repository contains selected 56Fe experimental-comparison tables and stage artifacts derived from the EXFOR experimental nuclear-reaction data system [6,7]. The Stage 24B summary identifies its computed inputs as preserved Stage 23C ECIS output tables, not output regenerated through the verified Python reference-calculation path. Because the public ECIS adapter is unavailable/experimental and host-dependent, these tables are historical evidence only; the ECIS reference is cited solely for historical context [8]. During Phase 1, the relevant files were inspected and their counts were checked, but the full acquisition, normalization, transformation, calculation, and comparison pipeline was not regenerated end to end.

The preserved comparison inventory contains:

Quantity	Preserved count
Total comparison rows	19,699
Interpolated rows	19,592
Rows matched at the same energy or angle without interpolation	107
Integrated-elastic rows matched at the same energy without interpolation	35

These counts are provenance facts about the preserved products. They are not an unqualified conclusion of experimental validation.

Observed discrepancies in energy regions with structure may be consistent with limitations of a smooth average optical potential, but no resonance-level analysis was performed. That possibility must not be stated as a demonstrated explanation.

Any quantitative residual, ratio, chi-square, or uncertainty statement used in a publication must be traced to its exact dataset, filtering rules, matching method, units, and executable analysis. The verified repository evidence does not establish complete covariance treatment.

7. Known limitations and reproducibility boundary

7.1 Scientific limitations

- The YOMS system description is general, while the verified numerical evidence in this edition is limited to the neutron-induced 56Fe worked example through the Python path, using the KD2003 functional form with the YOMS mass-derived $E_F = -9.4218 \ \ MeV$ convention.
- The global RIPL record-2405 expression gives $E_F = -9.79964 \ \ MeV$ for $A = 56$; this difference changes every energy-dependent potential depth. Internal YOMS regression is not exact evaluated-parameter identity with the global retrieval.
- Regression reproduction does not establish numerical convergence with respect to radial step, matching radius, or maximum partial wave.
- The standard test suite does not demonstrate broad reaction-channel validation.
- Preserved experimental comparison products were not regenerated end to end during Phase 1.
- No complete covariance or uncertainty-propagation workflow was verified.
- The potential-form sign and spin normalization were found consistent with the audited KD2003/RIPL conventions after the documented $U = -S$ transformation; this does not validate the chosen Fermi-energy convention or the numerical solution.
- No claim of superiority, universal convergence, general physical validity, or unrestricted predictive accuracy is supported.

7.2 Computational and portability limitations

- Only Darwin 25.5.0 on arm64 with CPython 3.14.0 was tested; the Phase 1 record did not capture NumPy, SciPy, or Matplotlib versions.
- Editable installation is not a verified workflow.
- ECIS06 is host-dependent, and the public ECIS adapter is not operationally documented.
- TALYS and SCAT2000 are placeholders.
- Selected frozen hashes do not certify the full repository, interpreter, dependency wheels, operating system, or external databases.

7.3 Publication and access limitations

This manual is published solely to document the scientific purpose, mathematical formulation, computational workflow, inputs, outputs, validation evidence, and limitations of the Yemeni Optical Model System (YOMS).

The YOMS source code, executable files, internal datasets, third-party software, and development repository are not distributed with this manual and are not made publicly available through the NATEC website. Publication of this manual does not grant a software licence or permission to access, copy, modify, or redistribute YOMS or any associated third-party materials.

References to ECIS06, SCAT2000, TALYS, RIPL, EXFOR, and other external resources are provided solely for scientific attribution, methodological context, and reproducibility documentation. No ECIS06, SCAT2000, or TALYS executable; RIPL- or EXFOR-derived database file; third-party source file; or other external software or data component is incorporated into or distributed with the publicly released manual package.

The public URL and the manual-only access and non-distribution boundaries are recorded in this edition. Any later change to the institutional rights statement or availability wording requires authorization by the National Atomic Energy Commission (NATEC). The scientific scope, documented capabilities, and limitations of YOMS are defined in this manual.

8. Troubleshooting

Import fails from outside the repository root

Return to the repository root and run the documented commands there. Do not substitute editable installation as though it had been verified.

Calculated values differ

Check:

1. host and architecture;
2. Python, NumPy, and SciPy versions;
3. working directory;
4. repository commit and dirty-tree status;
5. target mass and energy units;
6. potential name and backend;
7. protected-file verification; and
8. numerical settings in the frozen solver source.

Do not widen a tolerance merely to obtain a pass. Determine whether the difference is environmental, numerical, or scientific.

Frozen-core verification fails

Treat a mismatch as a provenance failure until the cause is identified. Do not overwrite protected artifacts merely to match a new result.

ECIS does not run

This manual does not describe the public ECIS adapter as operational. The bundled executable is host-dependent and may be incompatible with the current system. Do not use ECIS failure to infer failure of the verified Python workflow.

TALYS or SCAT2000 cannot calculate

They are placeholder backends in this snapshot. Registration does not imply calculation capability.

9. Protected assets and change control

The repository marks a selected frozen core in frozen_scientific_core/SHA256SUMS.txt. The verifier checks 430 entries. Before interpreting a regression:

1. record commit and dirty-tree state;
2. run the frozen-core verifier;
3. preserve changed inputs separately;
4. do not silently regenerate protected reference outputs; and
5. document any accepted scientific change with reviewer identity and rationale.

The frozen-core mechanism is an integrity aid, not a substitute for versioned release archives, dependency locks, data provenance, licensing review, or scientific peer review.

10. Conclusion and future scope

YOMS v1.0 provides a system-level technical framework for optical-model calculations of neutron-induced reactions. It records the governing mathematical formulation, optical-potential conventions, calculation organization, result interpretation boundaries, and reproducibility controls applicable to the documented system. In this edition, neutron-induced 56Fe is presented as the verified worked example: its KD2003-form potential, YOMS mass-derived Fermi-energy convention, evaluated parameters, preserved regression values, and provenance information provide a concrete demonstration of how a YOMS calculation is inspected and repeated.

The evidence establishes reproducible software behavior and numerical regression within the recorded boundary. It does not, by itself, establish universal numerical convergence, complete uncertainty quantification, unrestricted predictive validity, or exact evaluated-parameter identity with the global RIPL OMP record-2405 retrieval. Those questions require independent calculations, qualified nuclear-physics review, and comparison with traceable experimental data.

This manual serves as the citable system-level description of YOMS v1.0, with 56Fe as the verified worked example supplied in this edition. The use of 56Fe as the worked example in this edition does not limit YOMS to iron. YOMS is designed as a general computational framework for neutron-induced optical-model calculations and may be applied to other nuclides.

11. References

The following list is de-duplicated and cross-checked against the repository reference set in papers/56Fe_First_Paper/YOMS_Full_Manuscript_References.bib and publisher metadata. The repository BibTeX gives the Koning–Delaroche DOI with “(03)” in the suffix; the publisher record gives “(02),” which is used below. This discrepancy must be corrected in the authoritative bibliography after author review. DOI metadata should receive a final author proof before publication.

1. G. R. Satchler, *Direct Nuclear Reactions*, Clarendon Press, Oxford (1983).
2. R. G. Newton, *Scattering Theory of Waves and Particles*, 2nd ed., Springer-Verlag, New York (1982). https://doi.org/10.1007/978-3-642-88128-2.
3. R. D. Woods and D. S. Saxon, “Diffuse surface optical model for nucleon-nuclei scattering,” *Physical Review* **95** (1954) 577–578. https://doi.org/10.1103/PhysRev.95.577.
4. A. J. Koning and J. P. Delaroche, “Local and global nucleon optical models from 1 keV to 200 MeV,” *Nuclear Physics A* **713** (2003) 231–310. https://doi.org/10.1016/S0375-9474(02)01321-0.
5. R. Capote et al., “RIPL—Reference Input Parameter Library for calculation of nuclear reactions and nuclear data evaluations,” *Nuclear Data Sheets* **110** (2009) 3107–3214. https://doi.org/10.1016/j.nds.2009.10.004.
6. N. Otuka et al., “Towards a more complete and accurate experimental nuclear reaction data library (EXFOR): international collaboration between nuclear reaction data centres,” *Nuclear Data Sheets* **120** (2014) 272–276. https://doi.org/10.1016/j.nds.2014.07.065.
7. V. V. Zerkin and B. Pritychenko, “The experimental nuclear reaction data (EXFOR): extended computer database and Web retrieval system,” *Nuclear Instruments and Methods in Physics Research A* **888** (2018) 31–43. https://doi.org/10.1016/j.nima.2018.01.045.
8. J. Raynal, “Notes on ECIS94,” CEA Centre d’Études de Saclay report CEA-N-2772 (1994). Historical-context citation only; the authoritative report record remains pending confirmation.
9. A. J. Koning, S. Hilaire, and S. Goriely, “TALYS: modeling of nuclear reactions,” *The European Physical Journal A* **59** (2023) 131. https://doi.org/10.1140/epja/s10050-023-01034-3.

10. G. K. Sandve, A. Nekrutenko, J. Taylor, and E. Hovig, “Ten simple rules for reproducible computational research,” *PLoS Computational Biology* **9** (2013) e1003285. https://doi.org/10.1371/journal.pcbi.1003285.
11. M. D. Wilkinson et al., “The FAIR Guiding Principles for scientific data management and stewardship,” *Scientific Data* **3** (2016) 160018. https://doi.org/10.1038/sdata.2016.18.

Appendix A: Exact outputs, acceptance values, and hashes

A.1 Exact 0.8 MeV values

The verified Python result at $E_{lab} = 0.8 \ \ MeV$, using the frozen YOMS mass-derived $E_F = -9.4218 \ \ MeV$ convention, is:

Observable	Value (b)
Elastic	1.7964548678381935
Reaction	2.283992787174775
Total	4.080447655012969

The closure difference $\sigma_{tot} - (\sigma_{el} + \sigma_R)$ is zero for the stored values because total_b is defined by that sum.

A.2 Regression acceptance

tests/test_fe56_regression.py uses an absolute comparison delta of $5 \times 10^{-11} \ \ b$ for the selected integrated cross sections. This is the verified regression tolerance.

A.3 Selected SHA-256 evidence

Artifact	SHA-256
tools/calculate_fe56_koning_delaroche.py	30e407595090d29ebd9874ae2cf71604fde53ced551defbfe78283039bf2fd1f
resources/benchmarks/stage1_parameters/ benchmark_stage1_parameters.csv	aa6037b9c5a333507fb1c6f44a6afb21403b4f895c61612b69173de18b988301
resources/benchmarks/stage4_full_kd/ benchmark_stage4_full_kd.csv	b4a875b37a54d42bebf0da844d3a9530458427a1478c8123b13d7c5b4a0a6af7
resources/benchmarks/stage5_scat2000/ benchmark_stage5_scat2000_cross_sections.csv	9a3f199c1e143a5ce1b955df25db96bd7309b16f8c2d2b70cec7c9faadad5cd1
resources/benchmarks/stage6_exfor_comparison/ benchmark_stage6_exfor_comparison.csv	1c911a8b75ac66158f60af831373c7213ba8109f66e85afbfade5d38bc380a99
resources/benchmarks/stage7_talys/ benchmark_stage7_talys_comparison.csv	8f0830d4c9f8a1968df67045781737a8039e1aa537d9f067b7963e4947f84ec3

The corresponding repository-relative paths are controlled by frozen_scientific_core/SHA256SUMS.txt and the Phase 1 audit. A copied digest without its path is not sufficient provenance.

Appendix B: Repository and evidence map

Manual subject	Primary repository evidence	Verification evidence or reference
Public API and result structure	modern_omp/api.py; modern_omp/core/results.py; modern_omp/__init__.py	Phase 1 software-verification record
Nuclear-system inputs	modern_omp/core/nuclei.py; modern_omp/core/particles.py; modern_omp/core/reactions.py	examples/fe56.py
KD2003-form YOMS implementation and Fermi-energy distinction	modern_omp/potentials/koning_delaroche.py; tools/calculate_fe56_koning_delaroche.py; resources/RIPL3/optical/om-get/om-parameter-u.dat; resources/RIPL3/optical/om-get/om_retrieve.f	tests/test_fe56_regression.py for internal reproduction; [4], [5] for published/global conventions
Woods–Saxon forms	modern_omp/potentials/woods_saxon.py	source inspection; [3]
Kinematics and S matrix	modern_omp/solvers/smatrix.py	examples; regression test; [1], [2]
Integrated cross sections	modern_omp/solvers/cross_sections.py	examples/fe56.py; tests/test_fe56_regression.py
Frozen reference path	tools/calculate_fe56_koning_delaroche.py	tools/verify_frozen_core.py; frozen_scientific_core/SHA256SUMS.txt
Experimental comparison	resources/exfor/56Fe; resources/validation/stage24B/56Fe; tools/plot_fe56_elastic_exfor.py	preserved counts; [6], [7]
Backend status	modern_omp/backends; modern_omp/backends/__init__.py	Phase 1 source inspection and execution record
Package identity and declared license	pyproject.toml	Phase 1 metadata inspection
Bibliography	papers/56Fe_First_Paper/ YOMS_Full_Manuscript_References.bib	normalized reference list in Section 11

This appendix is a navigation map, not proof that every listed file has been independently validated.

Appendix C: Reproducibility checklist

- [ ] Work from the repository root.
- [ ] Record date, host, architecture, and operating system.
- [ ] Record Python and dependency versions.
- [ ] Record commit identifier and dirty-tree status.
- [ ] Verify the selected frozen-core manifest.
- [ ] Use neutron, 56Fe, the KD2003-form provider with the YOMS mass-derived Fermi-energy convention, and backend python.
- [ ] Record $E_F = -9.4218\ MeV$ as the YOMS convention and do not relabel the result as an exact global record-2405 retrieval.
- [ ] Preserve exact commands, stdout, stderr, and exit codes.
- [ ] Compare the 0.8 MeV results with Appendix A.
- [ ] Apply only the verified regression tolerance where the test defines it.
- [ ] Label preserved comparison products as not regenerated end to end.

- [ ] Distinguish coordinate matching from numerical agreement.
- [ ] Avoid claims beyond the defined scientific and computational scope.
- [x] Record authorship, citation, rights, public access, and availability boundaries for this publication.

Appendix D: Publication, rights, and scientific-review boundaries

D.1 Authorship and institutional record

The sole-author identity, institutional affiliation, corresponding-author contact, absence of ORCID, funding statement, acknowledgments, and conflict-of-interest declaration were supplied by the author on 2026-07-16.

The final publication record is governed by the following institutional conditions:

1. This public package contains the manual only; YOMS source code, executable files, internal datasets, and development repositories are not distributed.
2. References to ECIS06, SCAT2000, TALYS, RIPL, and EXFOR are provided for scientific attribution and methodological context; no third-party software or database is redistributed.
3. The public access point for this edition is the NATEC webpage at https://natec-ye.org/yoms/.
4. No DOI is assigned to this edition; the stable NATEC webpage is the cited access point.
5. Publication of the manual grants no software licence or permission to access, copy, modify, or redistribute YOMS or associated third-party materials.
6. The author remains responsible for the scientific content and for the interpretation boundaries stated in this manual; bibliography limitations are reported in Section 11.

D.2 Statements requiring qualified nuclear-physics review

1. The scientific justification for selecting the YOMS mass-derived $E_F = -9.4218 \ MeV$ convention instead of the global record-2405 expression.
2. Whether the implementation should retain its current identity wording or use a separately named convention in the associated paper.
3. The appropriateness of the mass, frame, and nonrelativistic kinematic conventions for the stated use.
4. The neutral asymptotic matching convention and matching-radius adequacy.
5. Partial-wave truncation, numerical convergence, and interpretation of $1 - |S_{\ell j}|^2$ as the reaction contribution.
6. The relationship between the Python results and an independently executed KD2003 or external-solver reference.
7. Independent physical validation and the physical interpretation of residuals in preserved comparison products.
8. The limited statement that discrepancies may be consistent with a smooth average optical-potential limitation, given that no resonance-level analysis was performed.
9. Any proposed uncertainty, covariance, goodness-of-fit, or validation conclusion.
10. The appropriate authoritative citation for the implemented Numerov recurrence, because the repository bibliography does not currently supply one.

D.3 Public access, provenance, and rights record

1. The version identifier, publication date, author, affiliation, and public URL are recorded in the front matter.

2. The manual distinguishes system-level capability from the target-specific verification evidence demonstrated for 56Fe.
3. The public package excludes YOMS code, executables, internal datasets, development repositories, and third-party software.
4. A SHA-256 manifest accompanies the local publication package so that the uploaded PDF can be checked against the approved master.

The scientifically defensible conclusion remains limited to reproducible software behavior and bounded regression evidence in the recorded environment; the specialist scientific-review items in Section D.2 remain explicit limitations rather than publication claims.

Appendix E: Technical coefficient, convention, and equation evidence

E.1 Literal-coefficient unit audit

The units of every literal coefficient in Equations (33)–(44) are:

Equation	Literal coefficients and units
(33), V_0	59.3 MeV; 0.024 MeV per unit A; 21 MeV multiplying dimensionless η
(33), v_1	0.007228 MeV^{-1}; 1.48×10^{-6} MeV^{-1} per unit A
(33), v_2	1.994×10^{-5} MeV^{-2}; 2.0×10^{-8} MeV^{-2} per unit A
(33), v_3	7.0×10^{-9} MeV^{-3}
(34)	1.3039 fm and 0.4054 fm
(35)	0.6778 fm and 1.487×10^{-4} fm per unit A
(36), A_V	12.195 MeV and 0.0167 MeV per unit A
(36), B_V	73.55 MeV and 0.0795 MeV per unit A
(38), A_D	16 MeV and 16 MeV multiplying dimensionless η
(38), C_D	0.018 MeV^{-1} and 0.003802 MeV^{-1}; 156 and 8 are dimensionless mass-number scales
(38), B_D	11.5 MeV
(39)	1.3424 fm and 0.01585 fm
(40)	0.5446 fm and 1.656×10^{-4} fm per unit A
(41)	5.922 MeV; 0.003 MeV per unit A; 0.004 MeV^{-1}
(42)	1.1854 fm; 0.647 fm; 0.59 fm
(43)	-3.1 MeV and 160 MeV

E.2 Detailed convention and numerical cross-check log

Comparison	Result at 0.8, 1.0, and 2.0 MeV	Interpretation
Active package kd2405_parameters versus frozen kd_parameters	Maximum absolute difference: 0.0 for all 15 fields	Exact binary equality is expected because the default 56Fe package path delegates to the frozen function. These are not independent implementations for this scope.
Active package versus Stage 1 primary parameter columns	Maximum absolute difference: $4.781952611665474 \times 10^{-12}$ MeV, for V at 1.0 MeV	Difference is limited to Stage 1 CSV decimal serialization. No value was adjusted to hide it.
Stage 1 primary columns versus Stage 1 ripl_ columns	Zero difference at the serialized precision for all selected rows and mapped fields	Both column groups use the YOMS mass-derived $E_F = -9.4218$ MeV convention. Their agreement is internal regression evidence and does not establish identity with a global record-2405 retrieval.
YOMS frozen depths versus global-record-expression depths	Nonzero differences occur for all five energy-dependent depths at 0.8, 1.0, and 2.0 MeV; see Section 3.9.5.	The Fermi-energy choice changes the evaluated depths. Preserved YOMS values must be identified by their convention.
Shared geometries	Stage 1 has one rw/aw pair and one rso/aso pair; package and frozen objects expose separate rwv/awv and rwso/awso fields	The active code sets $r_{WV} = r_V$, $a_{WV} = a_V$, $r_{WSO} = r_{VSO}$, and $a_{WSO} = a_{VSO}$. This is a schema difference, not a numerical disagreement.
Spin–orbit docstring versus execution	The frozen optical_strengths docstring mixes signed-potential and positive-strength conventions and labels the operator as unscaled $\mathbf{l} \cdot \mathbf{s}$. The executed function returns the positive-d term in S, while callers supply the eigenvalue of $\sigma \cdot \boldsymbol{l} = 2\boldsymbol{l} \cdot \boldsymbol{s}$.	The docstring is a documentation defect and is not authoritative evidence. Applying $U = -S$ to the executed expression yields Equations (29) and (30); no solver-sign defect was found by the convention audit.

The Stage 1 CSV also contains pre-serialization absolute-difference columns at floating-point roundoff scale for some rows. Those recorded differences do not change the selected serialized parameter values and are not reinterpreted here as physical uncertainty.

E.3 Complete equation-to-code evidence map

Equations	Implemented relation	Exact source file and function	Benchmark or regression evidence
(1)–(3)	Numerical reduced mass, frame conversion, and wave number with $m_u c^2$ explicit	tools/calculate_fe56_koning_delaroche.py: constants and s_matrix; modern_omp/solvers/smatrix.py: _kinematics	resources/benchmarks/stage4_full_kd/benchmark_stage4_full_kd.csv; tests/test_fe56_regression.py
(4)–(6)	Radial equation, $U = -S$, and local $q_{\ell j}$ with the atomic-mass conversion	tools/calculate_fe56_koning_delaroche.py: s_matrix and q_at; modern_omp/solvers/smatrix.py: neutron_s_matrix and q_at	Stage 4 benchmark; frozen-solver SHA-256 regression
(7)–(10)	Woods–Saxon, derivative surface, and full radii	tools/calculate_fe56_koning_delaroche.py: woods_saxon, derivative_shape, optical_strengths; modern_omp/potentials/woods_saxon.py: volume, derivative_surface	Stage 1 parameters; Stage 4 S matrix and cross sections
(11)–	Complex strength, spin–orbit	Executed optical_strengths in	KD2003 pp. 240–241, RIPL

Equations	Implemented relation	Exact source file and function	Benchmark or regression evidence
(14)	factor, pion length, and $\sigma \cdot \boldsymbol{I}$ eigenvalues	tools/calculate_fe56_koning_delaroche.py; kd2405_strength in modern_omp/potentials/koning_delaroche.py; callers in modern_omp/backends/python_solver.py; RIPL constants in resources/RIPL3/optical/om-get/om_retrieve.f	Handbook Eqs. (5.1)–(5.2), Stage 4 spin branches; docstrings are excluded as independent evidence
(15)–(18)	Neutral functions, matching ratio, S matrix, and transmission	tools/calculate_fe56_koning_delaroche.py: spherical_fg, s_matrix; modern_omp/solvers/smatrix.py: spherical_fg, neutron_s_matrix, SMatrixElement.transmission	Stage 4 S_real, S_imag, abs_S, and transmission_coefficient columns
(19)–(24)	Spin weights, integrated cross sections, closure, and units	modern_omp/backends/python_solver.py: _frozen_fe56_smatrix; modern_omp/solvers/cross_sections.py: integrate_cross_sections_with_k; frozen elastic_cross_section_b	Stage 4 cross-section columns; tests/test_fe56_regression.py; examples/fe56.py
(25)–(31)	Component potentials and total $U = -S$ mapping	optical_strengths in tools/calculate_fe56_koning_delaroche.py; kd2405_strength in modern_omp/potentials/koning_delaroche.py; solver q_at addition	Stage 1 component parameters; Stage 4 spin branches; KD2003/RIPL sign comparison
(32)	YOMS mass-derived Fermi and shifted energies	tools/calculate_fe56_koning_delaroche.py: FERMI_ENERGY, kd_parameters	Stage 1 parameter rows; distinct from the global expression in KD2003 Table 10 and RIPL record 2405
(33)–(44)	Energy-dependent depths and geometry	kd_parameters in tools/calculate_fe56_koning_delaroche.py; delegated package fields in modern_omp/potentials/koning_delaroche.py	Stage 1 primary and ripl_ columns at the selected energies

This inventory establishes implementation traceability and regression reproduction. The Phase 3B audit resolved the displayed potential-form signs and spin normalization against the inspected KD2003/RIPL conventions after the explicit $U = -S$ transformation. It does not establish numerical convergence, independent physical validation, uncertainty, or scientific interpretation.

اللجنة الوطنية للطاقة الذرية
NATIONAL ATOMIC ENERGY COMMISSION
NATEC

YOMS v1.0

User Manual and Reproducibility Guide

The Yemeni Optical Model System (YOMS) is an institutional scientific framework for organizing, executing, and documenting optical-model calculations of neutron-induced reactions. This manual records the mathematical formulation, computational workflow, inputs, outputs, verification evidence, reproducibility controls, and interpretation limits of YOMS v1.0.

SYSTEM SCOPE AND EVIDENCE

- YOMS is documented as a general system for neutron-induced optical-model calculations.
- Neutron-induced iron-56 (56Fe) is the verified worked example supplied in this edition.
- The worked example does not limit YOMS to iron; the system may be applied to other nuclides.
- Source code, executables, internal datasets, and third-party software are not distributed with this manual.

PUBLIC RECORD

https://natec-ye.org/yoms/

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