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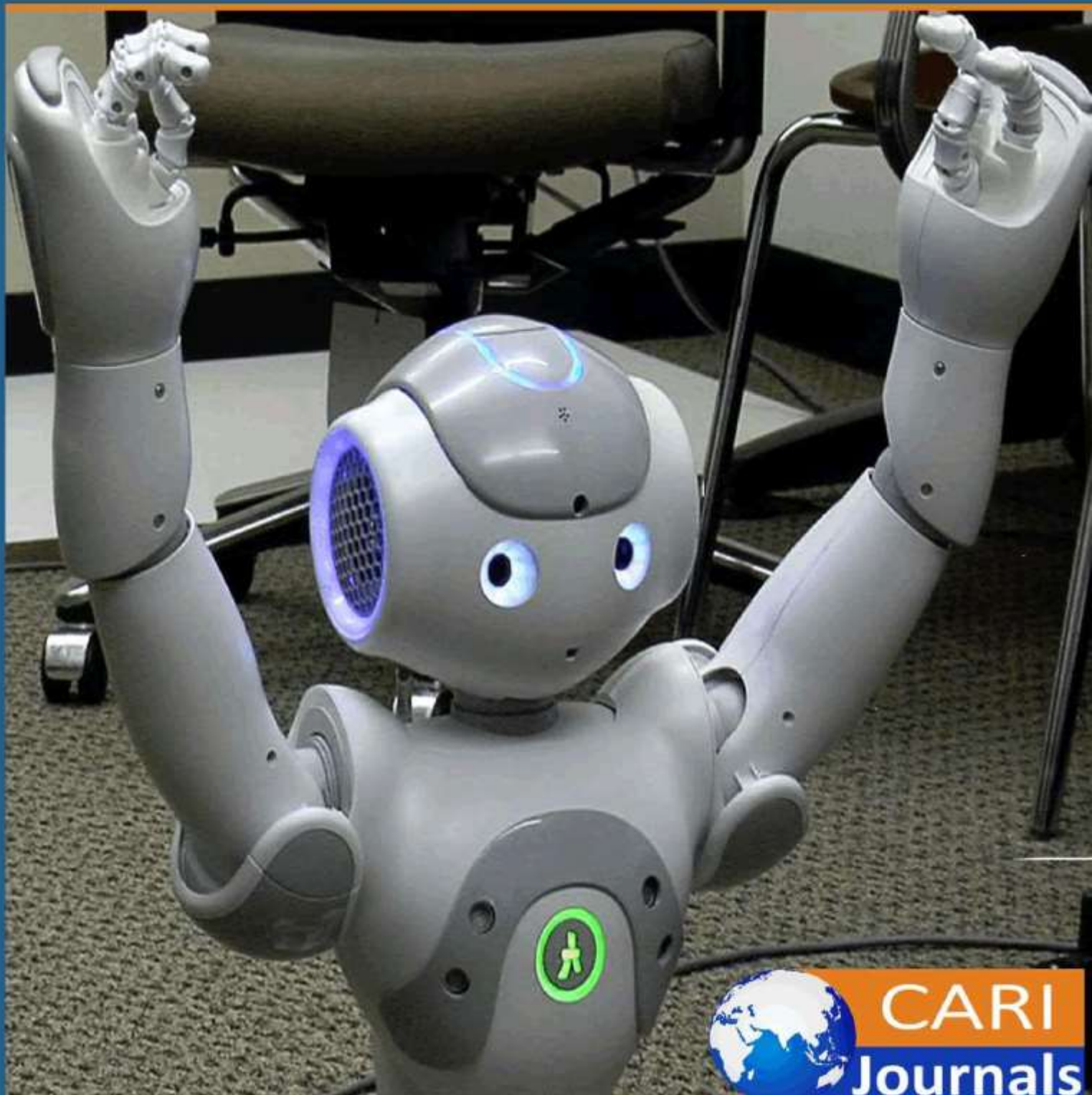

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Open-Source Modelling Tools in Chemical Engineering: Opportunities and Adoption in Malawi and Africa

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Abstract

Purpose: Computational modelling is central to chemical engineering education, research, and process design, yet sustained access to modelling capabilities in many low-resource institutions remains limited by high licensing costs and dependence on proprietary software ecosystems. This study examines the potential of open-source modelling tools to provide technically robust and institutionally sustainable alternatives, addressing persistent gaps in tool selection, curriculum integration, and long-term adoption.

Methodology: A systematic review and synthesis of open-source computational modelling tools across molecular, continuum, and process scales is conducted. Based on this analysis, a decision tree is developed to link modelling objectives and physical-fidelity requirements to appropriate open-source tools. In parallel, a decision-driven institutional adoption framework is proposed to guide phased implementation in resource-constrained chemical engineering environments.

Findings: The review shows that mature open-source tools now exist across the full modelling hierarchy, enabling core chemical engineering workflows without reliance on proprietary platforms. The proposed decision tree supports transparent and reproducible software selection, while the adoption framework highlights the central role of infrastructure readiness, skills development, curriculum maturity, and governance in sustaining open-source uptake. Explicit decision points and feedback loops are identified as critical for managing heterogeneous infrastructure and evolving human capacity.

Unique contribution to theory, practice and policy: This work delivers an integrated, decision-based approach to open-source modelling adoption in chemical engineering, linking technical capability with institutional capacity building. It provides actionable guidance for educators and institutions seeking equitable and sustainable digital modelling ecosystems, with relevance beyond the Malawian and Sub-Saharan African context.

Keywords: *Open-source modelling, Chemical engineering education, Computational modelling tools, Decision-support framework, Resource-constrained institutions*

Background

Computational modelling has become an indispensable component of modern chemical engineering. Whether in process simulation, molecular dynamics, atomistic simulations, or multiphysics modelling, computational modelling tools accelerate research, support design decisions, and enhance teaching. However, many traditional software packages, especially the commercial ones, carry significant licensing costs and ICT infrastructure demands that can limit their accessibility, especially in resource-constrained settings like Malawi and broader Sub-Saharan Africa. In this context, open-source computational modelling tools offer a viable opportunity for higher education and research institutions in Malawi and across Africa to democratise access to advanced modelling capabilities in chemical engineering.

Open-Source Software as an Enabler of Accessible Computational Modelling

Open-source modelling refers to developing and running scientific or engineering models using software whose source code is openly available, freely accessible, and legally modifiable (De Maria et al., 2020). In practice, it means that the tools, algorithms, solvers, and often full workflows are transparent, inspectable, and customisable by the user.

Open-source software offers several advantages. Firstly, it eliminates and/or dramatically reduces the cost barrier associated with proprietary licenses, enabling students and researchers to download and use powerful tools free of charge (Cummings & Gilmer, 2019). Furthermore, according to J.M. Pearce (2020), the use of open-source computational tools in scientific research generally leads to economic savings of up to 87% compared to when using proprietary tools. Beyond cost savings, open-source tools foster adaptability as users can modify code to fit their specific research or educational needs, thereby promoting innovation and a deeper understanding of modelling principles (Ansari et al., 2025). Moreover, research that has been conducted using proprietary software makes it hard to access the original code/model/script and this becomes problematic when other researchers are attempting to reproduce a computational study's results (Cummings & Gilmer, 2019). On the other hand, with open-source models, researchers can and usually upload the models onto open access repositories like GitHub where other researchers can easily access the models for reproducibility.

Across Africa, there is increasing advocacy for open science practices, reflected in a growing emphasis on open access publishing, open data, and the adoption of open-source software to support research, education, and institutional capacity building (Pienaar, 2023).

Barriers to Open-Source Adoption in African Higher Education

Although open-source tools have potential, their uptake in African higher-education institutions has been constrained by structural and systemic challenges. The African open science ecosystem still faces "huge gaps", most notably in e-infrastructure, institutional advocacy, and policy

adoption, which limit the full realisation of open-source benefits (Okafor et al., 2022; Skelly & Chiware, 2022).

Several empirical studies highlight the specific barriers that hinder the adoption of open-source modelling tools in Malawi and Africa. Firstly, poor ICT infrastructure and internet connectivity is seen as one of the most prohibitive barriers to realising an open-source chemical engineering modelling future. The internet capacity is uneven and often limited. Many African universities lack high-speed, reliable bandwidth, and must rely on low-bandwidth connectivity, which hampers online collaboration, software downloads, and remote learning (Ogunmakin, 2018). Furthermore, in Africa, technical weaknesses such as insufficient computer equipment, poor data security, and inadequate power supply have always been widespread in tertiary institutions (Samson Babalola & Akinyi Genga, 2024). More specifically in Malawi, studies of e-learning report that unreliable electricity supply is a key constraint: power outages affect students' ability to access digital resources (Gama et al., 2022).

Beyond poor ICT infrastructure, institutional policy and support also tend to hinder widespread support for the adoption of open-source scientific tools. Some universities lack coherent ICT strategies that explicitly support open-source software adoption. A review of ICT implementation in African universities, by Ntorukiri et al. (2022), found that weak institutional plans, underfunded ICT departments, and limited capacity to maintain hardware and software impede progress. Moreover, although there is increasing interest in open science, many institutions have not yet institutionalised open-source software in their policies or curricula, limiting practical adoption (Okafor et al., 2022).

Capacity shortage and lack of dedicated training on open-source software is another huge barrier to the future of open-source modelling in chemical engineering. There is a shortage of skilled personnel as many faculty and support staff in African universities lack the training and technical expertise needed to deploy, maintain, and teach with open-source modeling tools (Babalola & Genga, 2025).

According to Gownaris et al. (2022), a lack of advocacy and limited visibility of open-source science tools is one of the largest barriers to uptake. This problem is compounded by aggressive marketing, and/or popularity of proprietary software companies: many researchers in Africa may default to widely known commercial tools rather than explore open-source alternatives. Furthermore, institutional culture and legacy systems have also shaped how academic institutions view open-source software. Many academic departments are accustomed to proprietary software and may be resistant to transitioning to open-source alternatives. This resistance is not necessarily due to lack of will, but often reflects logistical inertia, lack of formal incentives, and concerns about support and stability. Institutions may also lack long-term strategic commitment; open-source projects may be seen as temporary or experimental rather than core to teaching and research infrastructure (Ntorukiri et al., 2022).

Finally, indirect financial and sustainability constraints present yet another challenge to the adoption of open-source modelling tools in chemical engineering and the scientific community altogether. While the software itself may be free, indirect costs remain significant since universities need to invest in infrastructure, training, system administration, and data storage (Kodhek & Kamau, 2025). This is further made worse due to limited funding for ICT and research in Africa explained earlier.

Rationale for a Review Focused on Malawi and Africa

Given the systemic barriers to accessing proprietary software and the growing technical maturity of open-source modelling tools, this review will provide a focused examination of chemical engineering open-source software within the Malawian and broader African context. The review will raise awareness among educators, researchers and institutional leaders about the range of freely available tools and how they can be integrated into chemical engineering teaching and research. It will also identify key capacity-building needs by highlighting gaps in training, infrastructure and institutional strategies that currently limit effective adoption. In addition, this review will serve as a call to action by outlining policy, educational and community-driven approaches to support sustainable uptake of open-source modelling. Finally, it lays the foundation for future empirical studies in Malawi and across Africa to evaluate adoption, usage, and educational or research impact.

Research Objectives

Based on the foregoing rationale, this review aims to systematically catalogue the major open-source computational tools used in chemical engineering and chemistry, including those applied to process simulation, molecular dynamics, thermodynamics, optimisation and multiphysics partial differential equation modelling. It further seeks to describe the capabilities, limitations and typical application domains of these tools. Building on this foundation, the review maps open-source alternatives to commonly used commercial chemical engineering software, such as Aspen Plus, COMSOL Multiphysics, ANSYS Fluent and MATLAB, and outlines realistic migration pathways for African institutions. In addition, the review assesses the current level of adoption of open-source tools across African universities by identifying documented case studies of successful integration as well as areas where uptake remains limited or absent. Finally, it proposes actionable, context-appropriate recommendations to enhance awareness, capacity building and sustainable use of open-source chemical engineering tools, and identifies the essential training and skills development needs required for students and researchers to effectively adopt, implement and maintain open-source computational tools within Malawian and broader African higher education systems.

Methodology for Identifying Relevant Literature and Tools

The literature search covered publications from approximately 2005 to 2025, reflecting the emergence and maturation of open-source computational tools in chemical engineering. To

systematically identify open-source modelling tools relevant to chemical engineering, as well as the literature assessing their capabilities, adoption and suitability for Malawian and African institutions altogether, we employed a structured, multi-stage methodology combining database searches, targeted keyword strategies and cross-verification with authoritative documentation and benchmarking studies. The approach followed principles from the PRISMA framework adapted for a software-focused scoping review (Page et al., 2021).

Literature Search Strategy

A comprehensive search was conducted across major academic databases, including Scopus, Web of Science, ScienceDirect and IEEE Xplore. Search queries drew on terms related to open-source modelling, chemical engineering simulation, process modelling, computational fluid dynamics, partial differential equation solvers, molecular and electronic structure modelling, numerical computing and software adoption in Malawi and Africa in general. Table 1 summarises the search strings employed in the literature identification stage.

Table 1. Keyword Groups and Search Strings

Keyword Group	Search Strings
Open-source modelling	"Open-source modelling"
Chemical engineering simulation	"Chemical engineering simulation tools"
Process simulation and CFD	"Process simulation" AND "open-source", "open-source CFD"
PDE solvers	"Open-source PDE solver"
Molecular modelling	"Molecular dynamics open-source"
Electronic-structure modelling	"DFT open-source"
Numerical computing	"Numerical computing open-source", "Python", "GNU Octave"
Software adoption in Malawi & Africa	"Software adoption Africa & Malawi" AND "engineering", "ICT Africa engineering education & Malawi"

These search strings ensured broad coverage across all relevant modelling scales addressed later in the review.

Inclusion and Exclusion Criteria

Screening of studies, technical documents and reports was conducted using predefined inclusion and exclusion criteria. Materials were included if they described or evaluated open-source computational tools applicable to chemical engineering, including broader open-source modelling

approaches, addressed tool capabilities, performance or typical application domains, discussed training, adoption, infrastructure or policy considerations relevant to African institutions, or provided methodological demonstrations, workflows or comparative analyses of modelling approaches. Items were excluded if they focused exclusively on proprietary software without comparative relevance, offered only superficial descriptions lacking methodological depth, or pertaining to fields unrelated to chemical engineering modelling.

Table 2: Criteria Applied During Screening

Inclusion Criteria	Exclusion Criteria
Open-source modelling discussions	Proprietary-only descriptions
Methodological or performance evaluation	Minimal methodological content
Relevance to chemical engineering domains	Irrelevant disciplinary focus
Discussion of adoption or training challenges	—

2.3. Identification of Software Tools

To ensure accurate identification of tools, information from the literature search was cross-verified using multiple authoritative sources. These included official documentation, update notes, community-maintained repositories, peer-reviewed benchmarking studies and reports discussing the adoption or use of modelling tools in chemical engineering education and research. This step supported the subsequent classification of tools and modelling domains presented later in the review.

Cross-Scale Mapping Procedure

Once the relevant tools and studies were identified, they were mapped onto modelling scales ranging from atomistic modelling to process-level simulation, including cross-scale numerical computing. The mapping was guided by several criteria, namely the underlying numerical or theoretical methods employed, the typical engineering applications associated with each scale, the input and output requirements of the tools, and their ability to interface with broader modelling workflows, including techno-economic assessment frameworks. This systematic mapping directly informed the modelling-scales and the structured domain classification used in the results and discussion sections.

African Contextualisation

Because the study focuses on Malawi and the wider African context, targeted searches were also performed using terms related to chemical engineering education, digital infrastructure and computational adoption challenges in African institutions. These additional searches helped contextualise the barriers and opportunities described in Section 1.2 and informed the interpretation of aggregated literature findings.

Validation and Triangulation

To improve reliability, all findings were cross-checked across multiple sources. Non-academic materials such as forums, blogs and community discussions were used only when they supported or clarified information found in peer-reviewed literature. Cost-related information for commercial software was confirmed, where possible, against vendor brochures or institutional licensing documents. This validation process ensured that the methodological synthesis remained transparent, reproducible and grounded in verifiable sources.

PRISMA Study-Selection Flow

The study-selection process involved several screening stages that reduced the initial pool of retrieved records to the final set included in this review. After compiling all records from database searches, documentation sources and grey literature, duplicates were removed and the remaining items were screened by title and abstract. Full-text assessment was then carried out using the predefined inclusion and exclusion criteria described earlier. This stepwise process ensured that only studies with clear methodological relevance to open-source modelling in chemical engineering were retained. The numbers corresponding to each stage of identification, screening, eligibility assessment and final inclusion are summarised in Figure 1.

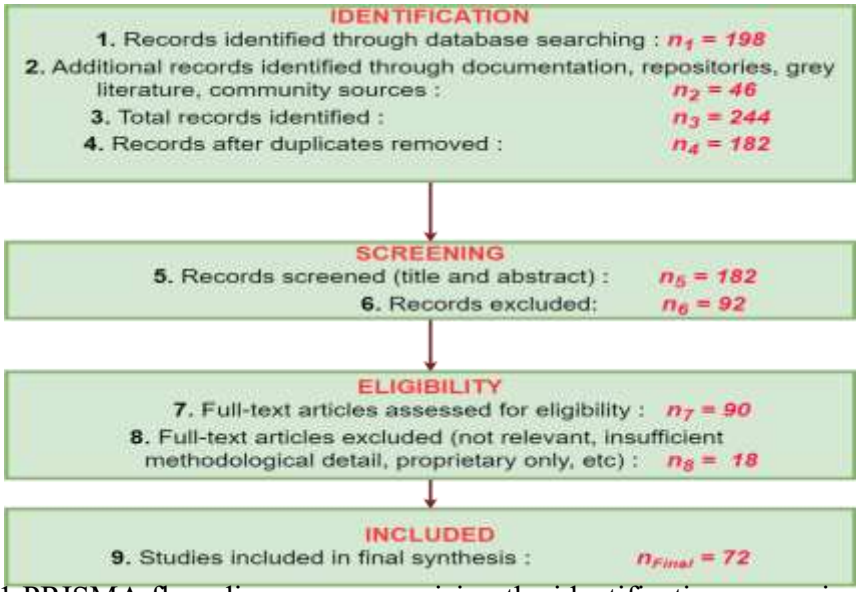

Figure 1 PRISMA flow diagram summarising the identification, screening, eligibility assessment and final inclusion of studies considered in this review.

Results

This section presents the outcomes of the systematic literature identification and classification process described in Section 2. The results focus on identifying open-source computational modelling tools that are actively used, documented, or discussed within the chemical engineering literature, and on organising these tools into coherent modelling domains. Rather than evaluating individual software packages in isolation, the results synthesise how open-source tools collectively span the full hierarchy of modelling scales encountered in chemical engineering education and research.

Modelling-Domain Classification of Open-Source Tools

The identified tools were grouped according to their primary modelling domains, ranging from atomistic and electronic-structure calculations, through molecular and mesoscale simulations, to continuum-scale transport modelling and process- and plant-level simulation. This domain-based organisation reflects how computational modelling is typically structured within chemical engineering curricula and research workflows, where tool selection is governed by the dominant physical phenomena, spatial and temporal scales, and intended application.

Table 3 summarises the principal open-source computational tools identified in the literature, together with their typical scopes of application and representative sources documenting their use. The table demonstrates that mature open-source alternatives now exist across all major modelling domains traditionally dominated by proprietary software, including process simulation and techno-economic assessment, computational fluid dynamics, multiphysics and partial differential equation solvers, molecular dynamics, electronic-structure modelling, electrochemical systems, and general scientific computing.

Table 3. Chemical Engineering Open-Source Computational Tools Classified by Modelling Domain

Modelling Domain	Main Tools Identified	Scope / Typical Applications	Source(s)
Process Simulation and Techno-Economic Assessments	DWSIM; COCO Simulator	Flowsheeting, thermodynamics, unit operations, equilibrium reactors,conversion reactors, process modelling	(Tangsriwong et al., 2020), (Oyegoke, 2023)
Computational Fluid Dynamics (CFD)	OpenFOAM	Laminar/turbulent flow, heat transfer, multiphase flow, reactive flow	(Chen et al., 2014)
Multiphysics / Partial Differential Equation (PDE) Solvers	FEniCS; FreeFEM++	Finite-element modelling of diffusion, heat transfer, electrochemical systems, fluid flow	(Alnæs et al., 2015a), (Pironneau, 2017)
Molecular Dynamics (MD)	LAMMPS; GROMACS	Classical mechanical atomistic simulations of materials, electrolytes, molecular interactions, transport properties	Thielemann et al., 2019)
Density Functional Theory (DFT) & Electronic Structure	Quantum ESPRESSO; GPAW; CP2K; NWChem	Quantum mechanical atomistic simulations to determine electronic structures, adsorption energies, catalytic surfaces, reaction pathways	(Giannozzi et al., 2009), (Larsen et al., 2017), (Valiev et al., 2010)
Thermodynamics & Chemical Reaction Engineering	Cantera; RMG-Py	Chemical kinetics, reaction mechanisms, combustion modelling, reactor simulations	(Goodwin et al., 2018), (Spiekermann et al., 2022)
Electrochemical Modelling	FEniCSx; FreeFEM++; PyBaMM	Electrochemical cells, Li-ion batteries, reaction–diffusion systems	(Molel & Fuller, 2023), (Orncompa et al., 2024), (Sulzer et al., 2021)
General Scientific Computing	Python (NumPy, SciPy, Matplotlib); GNU Octave	Numerical computation, optimisation, plotting, data processing, teaching workflows	(Molel & Fuller, 2023), (Hansen, 2011)
Geometry Preparation	FreeCAD	2D and 3D design and meshing of reactor geometries that are later exported to other software like FreeFEM++ or FEniCSx	(Riegel et al., 2016)

To complement the tabulated classification, Figure 2 presents a schematic representation of the modelling scales and domains associated with the identified tools. The figure illustrates how open-source tools are distributed across atomistic, mesoscale, macroscale, and process-level modelling, and how cross-scale scientific computing environments such as Python and GNU Octave support integration between these levels.

Together, Table 3 and Figure 2 provide a structured overview of the open-source modelling landscape in chemical engineering and establish the foundation for analysing tool capabilities, limitations, adoption patterns, and suitability for use in Malawi and other resource-constrained African contexts.

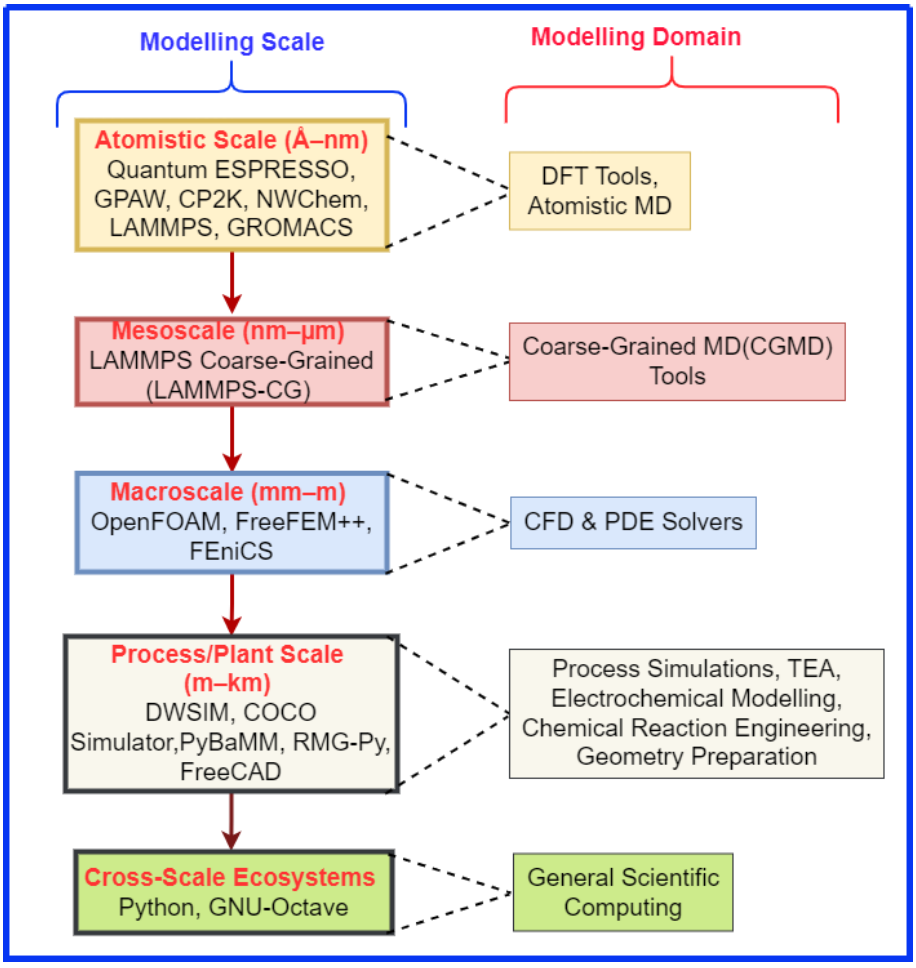

Figure 2: Modelling scales and domains of application of the open-source modelling tools identified in this study.

Capabilities and limitations across modelling scales

The open-source modelling tools identified in this study collectively span the full hierarchy of modelling scales shown in Figure 2, from electronic-structure calculations at the atomistic level to flowsheet-style simulations at the process and plant scale. At the atomistic scale (Å to nm), electronic-structure packages such as Quantum ESPRESSO, GPAW, CP2K, and NWChem operate within the density functional theory framework, solving approximate forms of the electronic Schrödinger equation to obtain equilibrium geometries, adsorption energies, reaction pathways, charge distributions, and related quantum-mechanical properties (Giannozzi et al., 2009; Larsen et al., 2017; Valiev et al., 2010). These tools are essential for studying catalytic surfaces, electrode–electrolyte interfaces, and molecular-level reaction mechanisms (Shan et al., 2017). Atomistic molecular dynamics tools such as LAMMPS and GROMACS simulate interacting atoms by integrating Newton's equations of motion (Thielemann et al., 2019).

Despite their high physical fidelity, atomistic approaches are constrained by small system sizes and short accessible timescales, typically on the order of femtoseconds (Kumar et al., 2022). Consequently, their primary role in chemical engineering lies in mechanistic understanding and in generating physically grounded parameters such as activation energies, adsorption strengths, and transport coefficients for use in higher-scale models (Manorosoa et al., 2025).

At the mesoscale (nm to µm), coarse-grained molecular dynamics implementations, particularly within LAMMPS, reduce atomic resolution by grouping atoms into interaction sites, enabling access to longer length and time scales while retaining essential physical behaviour (Thompson et al., 2022). Mesoscale simulations provide insight into interfacial phenomena, confinement effects, and effective transport properties that are difficult to represent using continuum approaches alone (Goh & Choi, 2025). Outputs from mesoscale modelling are frequently used to inform continuum-scale simulations through parameterisation of transport coefficients or interfacial behaviour (Bock et al., 2023).

At the macroscale (mm to m), OpenFOAM, FEniCSx, and FreeFEM++ provide continuum-level modelling capabilities based on conservation equations for momentum, heat, and species transport. OpenFOAM employs a finite-volume framework suitable for laminar and turbulent flow, multiphase systems, and reactive transport (Chen et al., 2014), while FEniCS/FEniCSx (Alnæs et al., 2015a; Molel & Fuller, 2023) and FreeFEM++ (Pironneau, 2017) offer finite-element environments that allow flexible formulation of coupled and nonlinear multiphysics problems. Although these tools are highly adaptable, they require substantial expertise in numerical methods, meshing, and solver configuration (Font & Peria, 2013), making them most appropriate for advanced teaching and research contexts.

At the process and plant scale (m to km), DWSIM, COCO Simulator, PyBaMM, and RMG-Py support flowsheeting, reaction engineering, and device-level electrochemical modelling. DWSIM and COCO provide steady-state and dynamic process simulation environments with

thermodynamic models, unit operations, and recycle handling suitable for mass and energy balance analysis and preliminary process design (Oyegoke, 2023; Tangsriwong et al., 2020). PyBaMM solves coupled electrochemical, diffusion, and charge-transport equations for battery systems (Sulzer et al., 2021), while RMG-Py generates detailed chemical kinetic mechanisms for reactor and combustion modelling (Spiekermann et al., 2022). FreeCAD supports geometry preparation for export to CFD and multiphysics solvers (Riegel et al., 2016).

Across all scales, Python and GNU Octave act as cross-cutting scientific computing environments supporting numerical computation, optimisation, automation, and reproducible workflows (Ford, 2014; Hagg & Kirschner, 2023; Zheng, 2023). Python-based ecosystems enable integration across modelling levels, including automation of electronic-structure calculations, post-processing of molecular dynamics trajectories, coupling with continuum solvers, and analysis of process-level simulations (Kluyver Thomas et al., 2016).

Mapping open-source alternatives to commercial software

The identified open-source tools can be mapped directly to widely used commercial chemical engineering software, revealing realistic migration pathways for academic institutions. Commercial platforms such as Aspen Plus/Aspen HYSYS, ANSYS Fluent/CFX, COMSOL Multiphysics, MATLAB, and SolidWorks remain dominant due to validated models, integrated workflows, and mature user support (Bartolome & Van Gerven, 2022; Chaurasia, 2021; Sharma & Gobbert, 2010). However, high licence costs, limited transparency, and dependence on proprietary ecosystems present significant barriers for many African universities (UNESCO, 2021).

In contrast, open-source alternatives DWSIM and COCO for process simulation, OpenFOAM and FEniCSx for transport and multiphysics modelling, LAMMPS and GROMACS for molecular simulation, Quantum ESPRESSO and related packages for electronic structure, Cantera and RMG-Py for kinetics, PyBaMM for electrochemical systems, Python and GNU Octave for numerical computing, and FreeCAD for geometry preparation collectively provide a coherent, licence-free modelling ecosystem suitable for teaching and early-stage research.

The literature consistently supports incremental rather than wholesale migration, in which open-source tools are introduced alongside commercial software for student projects and teaching laboratories, followed by deeper curriculum integration as capacity develops (Kluyver Thomas et al., 2016; UNESCO, 2021).

Extent and scale of adoption in African universities

Assessing the extent and scale of open-source modelling tool adoption in African universities is challenging due to the absence of systematic, tool-specific reporting in the peer-reviewed literature. Unlike commercial software, open-source tools are often adopted in decentralised and informal ways that are not captured by institutional audits. As a result, evidence consists primarily

of broad higher-education surveys of open-source software use (Tlili et al., 2022) and discipline-level case studies.

Documented case studies indicate adoption at the course or module level, such as the integration of FreeCAD and OpenFOAM into undergraduate engineering modules in South Africa (Botha & van Niekerk, 2025), demonstrating pedagogical viability. However, continent-wide, tool-resolved adoption metrics for chemical engineering departments are not currently reported, and this absence constitutes a key empirical finding of the review (Kamau & Namuye, 2012; Mwangi et al., 2021).

Discussion

This review demonstrates that the open-source chemical engineering modelling ecosystem is sufficiently mature to support teaching, research, and early-stage design workflows across molecular, continuum, and process scales (Alnæs et al., 2015b; Giannozzi et al., 2017). However, effective use in African universities is constrained less by software availability than by institutional capacity, staff training depth, and curriculum integration (UNESCO, 2021).

Decision tree for modelling tool selection

To support structured tool selection, Figure 3 presents a decision tree guiding users from problem definition to appropriate modelling domains and corresponding software options. The tree emphasises that modelling choices should originate from the engineering question rather than prior familiarity with specific software.

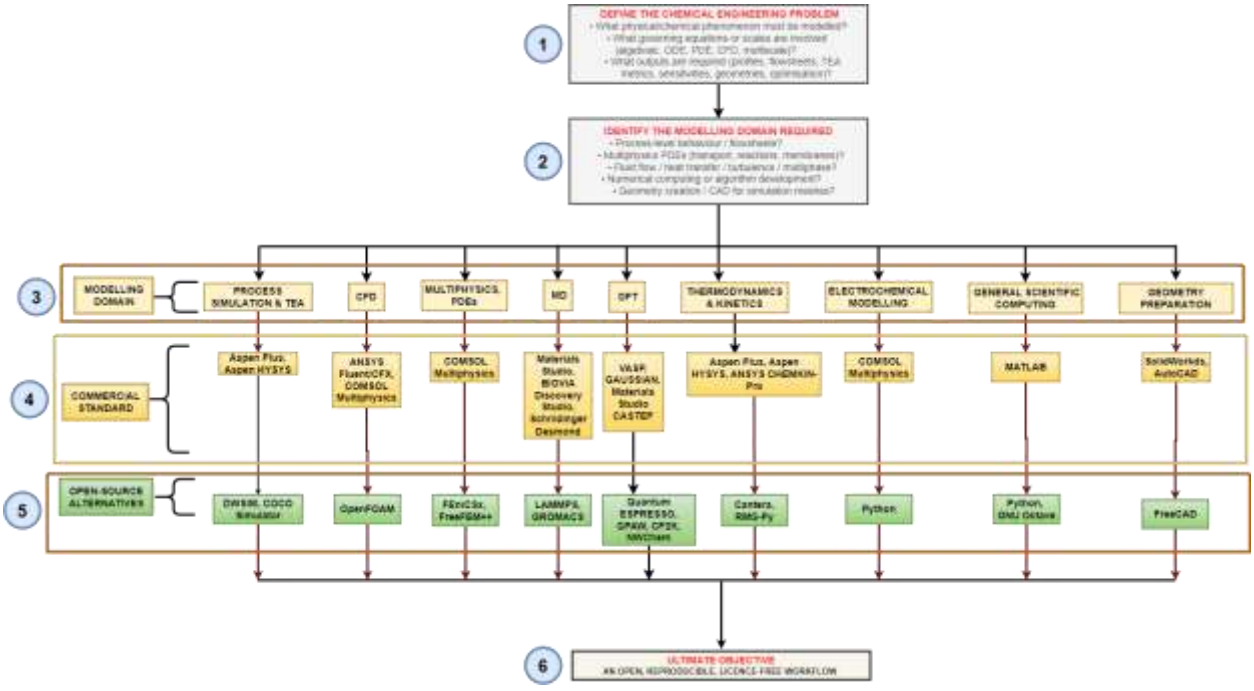

Figure 3 Decision tree for selecting chemical engineering modelling tools.

Decision-driven adoption framework

Building on the tool mappings and adoption challenges, Figure 3 presents a decision-driven framework for institutional adoption of open-source chemical engineering modelling. The framework conceptualises adoption as an iterative process governed by infrastructure readiness, skills adequacy, curriculum maturity, and institutional support, with remediation loops enabling staged capacity development.

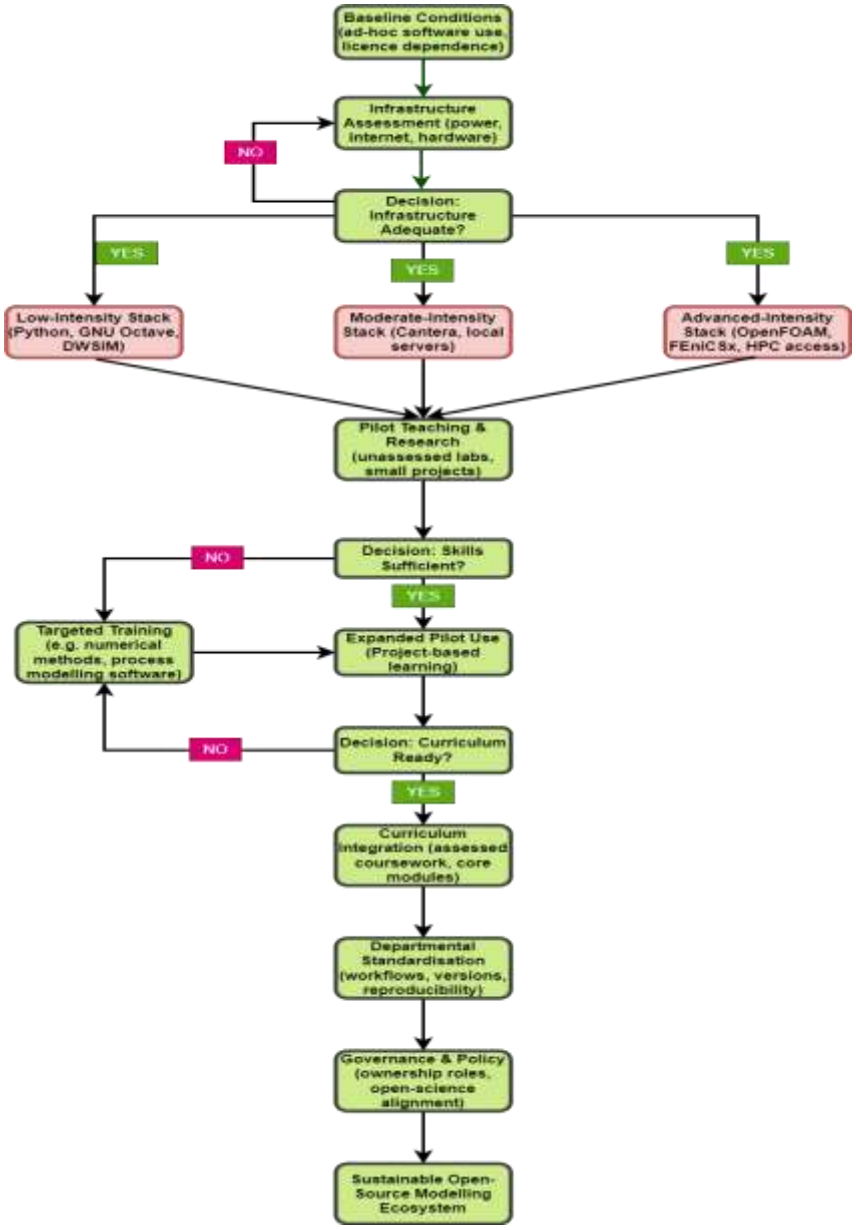

Figure 4: Decision-driven framework for institutional adoption

Actionable recommendations and skills requirements

Sustainable adoption requires curriculum-anchored integration, departmental workflow standardisation, explicit governance structures, local development of teaching materials, and recurring training programmes (Mengesha, 2010; Mwelwa et al., 2020a; Prince & Felder, 2006). Training must emphasise computational implementation of numerical methods, reproducible workflows, domain-specific modelling competence, problem formulation, and local technical support capacity.

Conclusions

This review examined the landscape of open-source computational modelling tools relevant to chemical engineering and evaluated their suitability for adoption in Malawi and other resource-constrained African institutions. By systematically mapping open-source alternatives to widely used commercial software across process simulation, computational fluid dynamics, multiphysics modelling, molecular simulation, electronic-structure calculations, electrochemical modelling, and numerical computing, the study demonstrates that technically credible and pedagogically validated open-source tools now exist across the full hierarchy of modelling scales encountered in chemical engineering education and research.

The findings indicate that there is no fundamental technical barrier to using open-source software for core chemical engineering modelling tasks. Mature platforms are available for flowsheeting and techno-economic assessment, continuum-scale transport and multiphysics simulation, atomistic and molecular modelling, and numerical computation. When combined within coherent workflows, these tools are capable of supporting undergraduate teaching, graduate-level research, and early-stage design and techno-economic analysis without reliance on proprietary licences.

However, the review also shows that adoption of open-source modelling tools in African universities remains uneven and insufficiently documented in the peer-reviewed literature. Evidence of adoption is primarily reported through qualitative case studies and general surveys of open-source software use, rather than through systematic, discipline-specific audits. While it is clear that adoption has occurred at least at the course or module level in parts of Africa, reliable continent-wide estimates of adoption within chemical engineering departments are currently unavailable. This limitation reflects gaps in reporting rather than an absence of implementation.

The analysis further demonstrates that sustainable adoption is driven less by software capability than by institutional and educational factors. Open-source modelling tools are most effective when they are formally embedded within curricula, aligned with assessment, supported by standardised workflows, and reinforced through recurring training. Numerical methods courses represent a particularly important leverage point, as coupling mathematical foundations with intensive computational practice enables students to develop transferable modelling skills that remain relevant beyond specific software platforms.

Overall, this study shows that open-source modelling tools provide a realistic and sustainable pathway for strengthening chemical engineering education and research in Malawi and similar resource-constrained contexts. The primary challenge is no longer access to capable software, but the deliberate and institutionally supported integration of computational modelling into routine academic practice. Addressing this challenge can reduce dependency on costly proprietary platforms, improve graduate preparedness, and support the long-term development of locally sustainable modelling capacity within African chemical engineering departments.

Author Contributions

Blessings G. Malimusi: Conceptualization, original idea development, study design, methodology development, data curation, literature searching and review, formal analysis, figure and table preparation, diagram creation, original scripting, writing---original draft, and manuscript editing.

Blessings G. Masina: Methodology contribution, literature searching, formal analysis, review, and manuscript editing.

All authors have read and approved the final manuscript.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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