Research on Hydrogen Redistribution in Xi' an Pulsed Reactor Based on RMC and COMSOL Platform

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Abstract

Reactor core simulation constitutes a critical component of nuclear reactor engineering design, encompassing multi-physics coupling processes including neutron transport and thermal-hydraulic phenomena. The Xi' an Pulsed Reactor (XAPR) employs uranium-zirconium hydride fuel, whose high-temperature hydrogen behavior significantly influences neutronic and thermal-hydraulic performance; however, investigations into the coupling between hydrogen migration and core physical characteristics remain inadequate. This study establishes a coupled neutronics-thermodynamics-hydrogen diffusion model for XAPR based on RMC Monte Carlo neutron transport simulations and COMSOL multi-physics simulations, investigating hydrogen redistribution patterns under the combined effects of temperature and concentration gradients. The results demonstrate that hydrogen diffusion behavior in zirconium hydride is synergistically regulated by temperature and concentration fields, with the redistribution process altering local hydrogen concentrations and consequently affecting neutronic performance and thermal-hydraulic characteristics. This research provides a theoretical basis for fuel optimization design and safety assessment of XAPR, and lays a foundation for hydrogen management strategies in reactors.

Full Text

Preamble

Study on Hydrogen Redistribution in the Xi'an Pulsed Reactor Based on RMC and COMSOL Platforms

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Abstract

Reactor core simulation is a critical component of nuclear reactor engineering design, encompassing multi-physics coupling processes such as neutron transport and thermal-hydraulic analysis. The Xi' an Pulsed Reactor (XAPR) employs uranium-zirconium hydride fuel, whose high-temperature hydrogen behavior significantly influences neutronic and thermal performance. However, research on the coupling effects between hydrogen migration and core physical properties remains insufficient. This study establishes a neutronics-thermodynamics-hydrogen diffusion coupling model for XAPR based on RMC Monte Carlo neutron transport simulation and COMSOL multi-physics field simulation to investigate hydrogen redistribution under the combined action of temperature and concentration gradients. Results demonstrate that hydrogen diffusion in zirconium hydride is co-regulated by temperature and concentration fields, and its redistribution alters local hydrogen concentration, thereby affecting neutronic performance and thermal-hydraulic characteristics. This research provides a theoretical basis for fuel optimization design and safety assessment of XAPR and lays the foundation for hydrogen management strategies in reactors.

Keywords: Xi' an Pulsed Reactor (XAPR); Metal hydride; Hydrogen redistribution; Multi-physics coupling; Monte Carlo simulation; Thermal hydraulics

Introduction

Reactor core simulation constitutes a core element of nuclear reactor engineering design. Nuclear reactor systems involve coupled multi-physics processes including neutron transport, fluid flow and heat transfer, and structural mechanics, which interact and synergistically determine reactor operational characteristics. High-performance computing-based multi-physics coupling simulation enables precise characterization of complex physical phenomena within the core and reveals the intrinsic mechanisms of reactor multi-physics coupling from first principles, which is crucial for enhancing reactor nuclear design and safety analysis capabilities [1-2].

The Xi'an Pulsed Reactor (XAPR) is a low-temperature, low-pressure pool-type pulsed reactor characterized by a small core size, strong neutron leakage, large local neutron perturbations, and highly non-uniform power and temperature distributions [3]. Conducting comprehensive safety analysis and evaluation is essential for ensuring safe XAPR operation and improving pulsed reactor safety levels [4].

In recent years, extensive research has been conducted on XAPR' s steady-state and transient operational characteristics. Despite these advances, several issues persist. First, isolated neutronics or thermal-hydraulic calculations fail to consider core interactions and coupling effects, inadequately reflecting actual XAPR operational processes. Second, existing neutronics-thermal coupling calculations rely on deterministic codes, requiring multi-group or few-group cross-section preparation for neutronics calculations that introduces significant approximations [5]. Meanwhile, XAPR employs uranium-zirconium hydride fuel whose high-temperature hydrogen behavior directly affects core neutron thermalization performance and thermal characteristics. Research indicates that hydrogen dissociation, migration, and redistribution in zirconium hydride, driven by temperature gradients, may cause local hydrogen concentration changes, significantly altering material neutron moderation capability and thermal conductivity. Huangs et al. [6] estimated hydrogen redistribution in zirconium hydride under temperature gradients through computational analysis; Yu et al. [7] employed machine learning molecular dynamics to simulate hydrogen diffusion pathways in ZrH , revealing temperature and composition effects on diffusion barriers; S. Yamanaka et al. [8] experimentally determined ZrHx thermal conductivity and expansion coefficients, establishing a hydrogen concentration-mechanical property correlation model. However, research on the coupling between hydrogen redistribution and neutronics/thermal characteristics in hydride fuel remains insufficient, hindering accurate assessment of operational hydrogen behavior and its feedback effects on reactor physical properties, which limits the accuracy of XAPR operational safety evaluation.

This study establishes a neutronics-thermodynamics-hydrogen diffusion coupling model for XAPR by integrating the RMC code [9] with COMSOL three-dimensional solid heat conduction and one-dimensional fluid single-channel heat transfer models. The model reveals hydrogen redistribution patterns under combined temperature and concentration gradients. Results demonstrate that hydrogen diffusion in zirconium hydride is influenced by both temperature and concentration fields, with redistribution significantly altering local hydrogen concentration and consequently affecting neutronic performance and thermal-hydraulic characteristics. This research provides theoretical support for XAPR fuel optimization design and safety margin assessment while establishing foundations for hydrogen management strategies in next-generation metal hydride-moderated reactors.

Methodology

1.1 RMC Calculation Model

For fuel rod power distribution calculations, this study employs the three-dimensional Monte Carlo neutron transport code RMC (Reactor Monte Carlo Code) independently developed by the REAL Team at Tsinghua University’ s Department of Engineering Physics [10]. The code accurately solves neutron flux density distribution by simulating random collisions between neutrons and nuclear fuel.

A full-core model is first established based on the pulsed reactor geometry, comprising 101 standard fuel elements. A refined spatial discretization strategy is then adopted—axially dividing into 10 layers and radially into 3 rings—to discretize the fuel region into 3,030 independent calculation units for precise power computation [11]. RMC tracks hundreds of millions of neutron histories, statistically determining interaction frequencies between neutrons and fissile nuclides (e.g., ^{235}U) in each unit. Combining pre-set nuclear database microscopic cross-section parameters, fission power density is calculated per unit according to P = R_f, where is the average energy released per fission and R_f is the fission reaction rate [12]. Finally, three-dimensional power distribution at the fuel rod scale is obtained through regional power density integration.

1.2 Thermal-Hydraulic Models

1.2.1 Solid Heat Transfer Model The solid heat transfer model adopts the classical steady-state heat conduction equation:

$$l \times - =$$

where l represents the thermal conductivity of fuel or cladding, and Q is the power density in the fuel region (W/cm^3).

The boundary condition at the cladding outer surface is a heat flux boundary:

$$- \times - =$$

where *T_{ext}* and h are the fluid temperature and convective heat transfer coefficient obtained from the one-dimensional fluid model, respectively, and n is the normal vector.

1.2.2 Single-Channel Model To simplify calculations and improve efficiency, this study employs a single-channel model for fluid analysis. The single-channel model is commonly used in reactor core thermal-hydraulic calculations, representing a simplified channel that reduces the core to a system comprising a single fuel rod and coolant channel, neglecting energy exchange with adjacent channels and considering only intra-channel energy transfer [14].

The axial temperature distribution of the fluid is solved using the energy conservation equation:

$$linear$$

where T is fluid temperature (K), z is axial height (cm), *P_{linear}* is linear power (W/cm), *c_p* is coolant specific heat capacity (J/(kg・K)), and *Q_m* is coolant mass flow rate (kg/s).

Derivation of the convective heat transfer coefficient involves parameters including fluid density (*(z)*), dynamic viscosity (*(z)*), and thermal conductivity (λ*(z)*). In this model, these three parameters can be obtained through temperature-dependent correlations. The relevant relationships are as follows:

where *v(z)* is coolant velocity at height z and s is the coolant channel radial area.

Based on this, the Reynolds number *Re(z)* can be calculated:

$$Re()()()$$

where d is the coolant channel equivalent diameter.

From this, the Prandtl number *Pr(z)* is obtained:

$$Pr()$$

The Peclet number *Pe(z)* is then calculated from Reynolds and Prandtl numbers:

$$RezPrz$$

Substituting into the heat transfer correlation for rod bundle channels yields the Nusselt number *Nu(z)*:

$$4.00.33(0.16($$

where p represents pitch and D represents fuel element outer diameter.

The heat transfer coefficient *h(z)* is then determined from the Nusselt number:

$$()()$$

1.3 Hydrogen Redistribution Mechanism

Compared to other hydrogen-containing materials, metal hydrides exhibit higher hydrogen density. Driven by temperature or concentration gradients, hydrogen can migrate and redistribute within hydrides, creating spatial concentration variations that subsequently affect neutron transport behavior and thermal-hydraulic characteristics in reactors. The analysis begins with thermal conduction calculations for fuel, moderator, and reflector regions using COMSOL' s built-in solid heat transfer module, with attention to contact thermal resistance between different materials—addressed herein using a conventional gas gap thermal resistance expression. After obtaining the fuel temperature field distribution, hydrogen diffusion and migration within the fuel are investigated.

Three effects govern hydrogen redistribution in metal hydrides: (1) concentration diffusion (Fickian effect), from high to low concentration regions; (2) thermal diffusion (Soret effect), from high to low temperature regions; and (3) stress effect, from highly compressed to highly tensile regions. The superposition of these three driving forces determines the hydrogen diffusion flux J_H, defined as:

$$= - +$$

where D is the hydrogen diffusion coefficient in the matrix, C is hydrogen concentration, *Q** is heat of transport, T is temperature (K), R is the gas constant, r is radial position, σ is stress gradient, and *V** is the volumetric expansion from solutes such as fission products or gases, resulting from lattice distortion or material deformation. Since stress gradient parameters in hydrides are relatively small, stress-driven diffusion is typically neglected in hydride diffusion modeling. Therefore, Equation (10) can be simplified to:

$$= - - DCD$$

where k_s is the Soret factor and $T\_\{abs\}$ is absolute zero.

This is implemented using COMSOL’ s coefficient-form partial differential equation module. Mass diffusion calculations require the previously computed temperature field as initial input to complete thermal and concentration diffusion. In metal hydrides, Soret effect-driven thermal diffusion and Fickian concentration diffusion produce opposing actions: temperature gradients induce Soret diffusion flux, creating hydrogen concentration imbalances that activate Fickian diffusion. Eventually, both diffusion effects reach equilibrium, resulting in zero net diffusion flux.

The overall structure of the multi-physics platform established in this study is shown in [Figure 1: see original paper]. During initial startup, RMC neutron calculations provide axial and radial power distributions, after which a new model is created through COMSOL’ s “Model Wizard.” The single-channel method requires creating two components under the same model: a one-dimensional fluid component and a three-dimensional solid component. Fluid calculations are implemented using COMSOL’ s coefficient-form PDE module, with axial power distribution input via “interpolation” functions to solve for coolant temperature and convective heat transfer coefficients required for three-dimensional heat transfer calculations. Following fluid calculations, a three-dimensional fuel rod geometry component is created, with heat transfer completed through the “Solid Heat Transfer” module. The external temperature and heat transfer coefficient in the boundary condition “Heat Flux” are manually passed via “interpolation” functions using the previously calculated fluid temperature and convective heat transfer coefficient, while power distribution is loaded through “analytic” functions using axial and radial power from neutron calculations. After obtaining the temperature field of the fuel rod component, hydrogen diffusion is calculated by adding a "Coefficient Form PDE" physics module. Post-calculation, the latest data are input into MCNP cards to update temperature and hydrogen fractions, yielding new power distributions for iterative computation until convergence is achieved.

Model Validation

2.1 UZrHx Fuel Pellet Validation

Focusing on key processes in hydride-moderated high-temperature reactors, this study investigates diffusion effects on multi-physics coupling mechanisms. To validate the established diffusion model, a standard fuel rod numerical model was constructed using the COMSOL multi-physics simulation platform based on classical experimental parameters from Huangs et al. (2000) [6]. The cylindrical fuel rod geometry was specified as radius 0.5 cm and height 1 cm, with an initial H/Zr atomic ratio of 1.6. Detailed calculation parameters are provided in . By applying a linear heat flux of 150 W/cm and a surface temperature boundary condition of 677°C, the three-dimensional temperature field of the fuel rod was successfully obtained.

Based on this temperature field data and material property parameters listed in , a hydrogen diffusion kinetics model for the UZrHx fuel system was established. Numerical simulation results in [Figure 2: see original paper] demonstrate that under temperature gradient driving, hydrogen atoms exhibit directional migration from the high-temperature core region toward the low-temperature surface region. The surface hydrogen concentration evolution over time is shown in [Figure 3: see original paper]. The computational results agree more closely with Huangs' classical experimental data [6] than with Mehta' s theoretical predictions [15]. When surface temperature reaches its minimum value, surface H/Zr increases continuously from the initial 1.60 to a steady-state value of 1.66, validating the diffusion model' s reliability under constant surface temperature boundary assumptions.

2.2 Nine-Rod Bundle CFD/Single-Channel Comparison

To systematically evaluate the computational accuracy and efficiency of the single-channel model in thermal-hydraulic analysis, a simplified 3$×$3 fuel assembly benchmark case was designed for comparison between full three-dimensional CFD simulation and one-dimensional single-channel simplified modeling. The case focuses on basic heat transfer characteristics under single-phase flow conditions, temporarily ignoring structural components such as grids and end fittings.

As shown in [Figure 5: see original paper], the fuel assembly consists of nine regularly arranged ZrH1.6 fuel rods in a square lattice configuration. Each fuel rod has a radius of 5 mm, pitch of 12 mm (P/D=1.2), and height of 5 cm. To simplify the computational domain, uniformly distributed linear heat flux (100 W/cm) is applied axially. Thermodynamic properties of involved materials are provided in , while relevant boundary conditions for the CFD thermal-hydraulic model are listed in .

For meshing, the CFD model employs a refined structured grid strategy, with the computational domain comprising 1,177,553 domain elements, 106,964 boundary elements, and 4,532 edge elements to ensure high-precision solution of fluid-structure coupling heat transfer problems. [Figure 6: see original paper] presents computational results from both CFD and single-channel models. Steady-state calculations based on the k-ω turbulence model required approximately 1,606 seconds in the computational environment. In contrast, the single-channel model using one-dimensional simplification requires only 100 axial nodes to characterize coolant channel heat transfer, with a single calculation taking only 15 seconds on the same hardware—representing a two-order-of-magnitude improvement in computational efficiency. Regarding accuracy, temperature distribution comparisons reveal a maximum relative deviation of only 1.6% between single-channel and CFD results. The study demonstrates that under single-phase flow uniform heating conditions, the single-channel model achieves highly consistent temperature field predictions (deviation <2%) at extremely low computational cost (<1% of CFD computational time).

Subsequently, hydrogen diffusion calculations were performed on the single-channel nine-rod bundle model. Figure 8: see original paper illustrates the relationship between radial temperature distribution and hydrogen concentration: temperature decreases gradually from the fuel pellet center toward the cladding surface radially, while hydrogen concentration exhibits the opposite distribution trend. This characteristic is closely related to hydrogen diffusion behavior in metals, as elevated temperatures accelerate hydrogen migration, resulting in reduced hydrogen concentration in high-temperature regions.

Figure 8: see original paper further demonstrates the axial temperature and hydrogen concentration distribution relationship. The axial temperature distribution exhibits typical parabolic characteristics, reaching maximum temperature at the fuel rod midplane and decreasing toward both ends. Correspondingly, hydrogen concentration is lowest at the fuel rod midplane and increases toward both ends. This "high temperature-low hydrogen concentration, low temperature-high hydrogen concentration" distribution pattern aligns perfectly with hydrogen solubility characteristics in metals, validating model reliability.

XAPR Analysis

3.1 XAPR Model Description

Following validation of the hydrogen diffusion and single-channel models, XAPR analysis calculations were performed. Based on the COMSOL multi-physics coupling platform, this study conducts multi-physics coupling analysis of XAPR under 2 MW steady-state operating conditions using an integrated modeling approach combining RMC Monte Carlo, three-dimensional solid heat conduction, and one-dimensional fluid flow heat transfer models.

The XAPR steady-state core layout is shown in [Figure 9: see original paper]. The core consists of 211 channels distributed across nine circles, with a central water cavity at the center and control rods occupying six channels. Within the core, 99 channels contain standard fuel elements, and two channels are designated for temperature measurement fuel elements. Additional core components include graphite elements, steady-state control rods, pulsed control rods, neutron source elements, absorber elements, and other relevant components. Notably, the two temperature measurement fuel elements labeled C10 and D2 in [Figure 9: see original paper] monitor core temperatures at power peaking locations during steady-state and pulsed operations. The temperature measurement fuel elements employ identical fuel structures as standard fuel elements.

The XAPR standard fuel element is illustrated in [Figure 10: see original paper]. The fuel element uses UZrH1.6 as fuel, with a central zirconium rod providing structural support. Helium gas at 0.1 MPa pressure fills the gap between fuel pellets and cladding. This helium filling enhances heat conduction between fuel pellets and cladding in addition to facilitating component leak testing [5]. Basic fuel element parameters are detailed in , with relevant physical properties for XAPR calculations provided in .

Based on the aforementioned model, the fuel rod section of XAPR was modeled in COMSOL. Free tetrahedral meshes with “finer” size settings were employed for model discretization as shown in [Figure 14: see original paper], with the complete mesh comprising 19,217,912 domain elements, 6,125,542 boundary elements, and 317,457 edge elements. Power loading adopts a “three radial rings, ten axial layers” division method [11], with each fuel rod divided into thirty sections totaling 3,030 regions.

3.2 Sensitivity Analysis

Hydrogen diffusion sensitivity analysis constitutes a crucial aspect of XAPR uranium-zirconium hydride fuel performance investigation. This study systematically examines the influence mechanism of transport heat Q on hydrogen redistribution through establishment of a single XAPR fuel rod model within the RMC-COMSOL collaborative simulation framework. While maintaining standard fuel rod dimensions (39 cm axial length, 1.805 cm radius) and constant rod power, multiple experimental datasets were synthesized to determine a reasonable Q value range. Based on Sommer and Dennison’ s classical experimental results [16], a baseline value of $Q = 5.3$ kJ/mol was selected. Considering Huang et al.’ s [6] finding that Q value variations within approximately 30% have limited impact on hydrogen distribution, a lower bound of $Q = 3.7$ kJ/mol was selected. Additionally, Merten et al.’ s theoretical model [17] was referenced to examine $Q = 2.1$ kJ/mol.

Computational results in [Figure 12: see original paper] demonstrate that transport heat Q significantly influences hydrogen redistribution behavior. As Q increases from 2.1 kJ/mol to 5.3 kJ/mol, the hydrogen atomic ratio (H/Zr) difference between fuel pellet center and cladding under steady-state conditions expands from 0.44 to 1.17, while time to reach steady state decreases from 5,730 days to 5,490 days. This phenomenon confirms positive correlation between Soret effect intensity and Q, where higher transport heat substantially enhances temperature gradient-driven hydrogen migration. Specifically, larger Q values indicate greater hydrogen atom sensitivity to temperature gradients, generating stronger thermal diffusion flux under identical temperature fields and resulting in more pronounced hydrogen redistribution and faster steady-state establishment.

3.3 Convergence Analysis

To achieve multi-physics coupling analysis of the XAPR system, the core region is divided into 3,030 independent units after obtaining temperature field and H/Zr distribution data from thermal-hydraulic and hydrogen diffusion calculations. Temperature and H/Zr values in each unit are updated zone-by-zone into material properties in the RMC input deck for recalculation. In neutronics calculations, 500,000 particles per generation are used, with 100 inactive generations to eliminate initial source distribution effects and 500 active generations for statistical convergence. The relative error tolerance for fuel rod heat conduction calculations is set at 1\$×10$^{\{-8\}, withcouplingiterationrelativeerrorat1\times10}${-4}\$.

As shown in , *k_{eff}* decreases to 1.01245 ± 0.00020 after the first coupling iteration, indicating that hydrogen migration exerts significant negative reactivity feedback. Meanwhile, maximum fuel temperature variation remains limited. Compared with initial uniform distribution assumptions, the post-redistribution physical field distribution is overall similar, with maximum temperature deviation of approximately 3% and maximum H/Zr concentration deviation of approximately 1.5%. This indicates that material nuclear cross-section parameter changes are not significant, and coupling calculations have essentially converged after one iteration. Therefore, under current accuracy requirements, multiple iterations between RMC neutronics calculations and COMSOL multi-physics simulations are unnecessary, demonstrating the effectiveness, computational efficiency, and numerical stability of the established coupling model.

3.4 Calculation Results

[Figure 13: see original paper] presents the core power parameter distribution under 2 MW steady-state operating conditions. Results reveal that fuel elements surrounding the central water cavity exhibit higher power density, primarily due to neutron moderation by the central water cavity. Overall power decreases radially from inside to outside within individual fuel rods, axially from midplane toward both ends, and globally from core center outward.

[Figure 14: see original paper] shows the radial temperature field at XAPR Z=0, [Figure 15: see original paper] illustrates the overall temperature distribution within core fuel rods, and [Figure 16: see original paper] displays temperature distribution in temperature measurement fuel element C10. Model accuracy is validated by comparing C10 temperature distribution with experimental values. Measurement point locations described in are as follows: #1, #2, and #3 are fuel temperature measurement points located at the radial center of C10 fuel rod, with #2 at the axial center and #1 and #3 positioned 2.5 cm above and below #2, respectively. Calculations show that the maximum temperature within C10 temperature measurement fuel element reaches 799.3 K, deviating from measured values by approximately 1.2%.

[Figure 17: see original paper] presents axial temperature distributions for different coolant channels calculated by COMSOL, where T_{coolant1} through T_{coolant10} represent coolant temperatures for the ten fuel rods in the row containing C10. Comparison with [Figure 14: see original paper] reveals that coolant temperature increases gradually from left to right, peaking at the fifth rod corresponding to maximum fuel rod temperature, then decreases progressively—consistent with power distribution trends.

[Figure 18: see original paper] shows the radial hydrogen redistribution field at XAPR Z=0, while [Figure 19: see original paper] presents hydrogen redistribution fields in core fuel rods at different calculation times (660 d, 5,850 d, and 6,150 d). Results indicate that as calculation time increases, hydrogen concentration nearly reaches steady-state distribution by 5,850 d, with maximum value reaching 1.96 and minimum value 1.46. Radially, hydrogen concentration is lowest at fuel rod center and increases toward the cladding surface; axially, hydrogen concentration is lowest at fuel rod midplane and increases toward both ends, consistent with the “high temperature-low hydrogen concentration, low temperature-high hydrogen concentration” distribution pattern.

Conclusions and Outlook

This study investigates XAPR steady-state power distribution, temperature distribution, and hydrogen redistribution based on RMC Monte Carlo neutron transport simulation and COMSOL multi-physics simulation. One-dimensional coolant and three-dimensional fuel rod power distributions were obtained through RMC calculations. Parallel integration of coolant single-channel and fuel rod three-dimensional heat conduction models enabled internal coupling computation via COMSOL, with hydrogen redistribution fields derived from temperature field calculations. Results demonstrate that hydrogen diffusion in zirconium hydride is co-regulated by temperature and concentration fields, with redistribution altering local hydrogen concentration and consequently affecting neutronic performance and thermal-hydraulic characteristics. It should be noted that for reactors like XAPR typically operating in one-to-two-hour full-power pulsed modes, significant hydrogen redistribution is unlikely to be observed during actual operation due to short operational durations; this phenomenon primarily occurs under prolonged continuous full-power operating conditions.

Worthy of further investigation is whether XAPR’ s characteristic pulsed operational mode, featuring periodic rapid temperature field variations with power pulses, could cause redistributed hydrogen to undergo reverse migration, partially or completely restoring its initial distribution. This issue involves coupling mechanisms between transient diffusion kinetics and thermal cycling effects, representing a key aspect of understanding pulsed reactor fuel behavior. Future work could combine transient thermal-hydraulic models with dynamic hydrogen diffusion simulation to deeply investigate pulsed operation effects on hydrogen distribution reversibility, providing more comprehensive theoretical support for pulsed reactor fuel lifetime assessment and safe operational strategies.

Consequently, the hydrogen redistribution patterns and their effects revealed in this study primarily serve to understand XAPR fuel behavior under extreme or long-term operating scenarios, while providing critical theoretical foundations for optimizing fuel design, conducting more comprehensive safety assessments, and establishing hydrogen management strategies.

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Note: Figure translations are in progress. See original paper for figures.