FUDMA Journal of Renewable and Atomic Energy (FJoRAE)
ISSN: 3027-2335
Vol. 3 (SI) 2026 Pp 1-9
DOI: https://doi.org/10.33003/fjorae.2026.03SI.77

Steady State Thermal Modeling and Heat Flux Analysis of Zinc–Calcium–Aluminosilicate (ZCAS) Glass-Ceramic Using COMSOL Multiphysics

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ABSTRACT
So, a three-dimensional steady-state thermal analysis of zinc–calcium–aluminosilicate (ZCAS) glass, basically a silicate-based material that people often value because it has strong thermal stability and structural reliability in engineering, also optical applications, was performed using the finite element method in COMSOL Multiphysics version 6.2. The Heat Transfer in Solids interface was selected to handle the steady-state heat conduction equation with mixed boundary conditions, meaning two isothermal surfaces plus the other boundaries were thermally insulated, but you know not all of them, just the remaining ones. The ZCAS glass itself was described as a homogeneous and isotropic solid, with density 2500 $kg \cdot m^{-3}$, thermal conductivity 1.20 $W \cdot m^{-1} \cdot K^{-1}$, and specific heat capacity 750 $J \cdot kg^{-1} \cdot K^{-1}$. A tetrahedral mesh, with 42,857 elements and 85,742 nodes was used, and yeah the mesh seemed to behave nicely. The computed results indicate a pretty smooth, almost monotonic temperature distribution with a maximum temperature difference of 17.2 K over the whole domain. The conductive heat flux vectors follow the main temperature gradient quite well, with a peak size around 860 $W \cdot m^{-2}$, so this is in line with Fourier's law of heat conduction. Then, a three-dimensional cut-line temperature profile shows a linear trend, which matches the analytical one-dimensional steady-state solution, and the relative errors stayed under 2.5%. Also, when integrating the normal total energy flux over the surfaces, the inlet gives 103.8 W and the outlet gives +103.8 W, so the energy imbalance is less than 0.7%. That basically confirms steady-state energy conservation, which you want to see of course. Overall, once the thermal model was checked, it suggests ZCAS glass maintains stable and predictable heat conduction behaviour even under moderate thermal gradients. These results back up that ZCAS glass is suitable in general, whether it comes from high-purity oxides, or from more sustainable waste-derived precursors, like recycled silica and calcium-rich waste streams, for optical components, electronic packaging, and thermal-resilient structural setups.

Keywords: Steady-state heat conduction, ZCAS glass, Finite element method, COMSOL Multiphysics, Heat flux, Energy conservation

1.0 INTRODUCTION

Modern engineering applications are using glass materials more and more, mainly because they give a kind of weird but useful mix of optical clarity, chemical resistance, and a thermal conductivity that can be controlled (or at least adjusted). Because of that, glasses end up in photonic devices, electronic packaging substrates, biomedical coatings, and even thermal barrier systems. And in these cases, you really need stable, predictable heat conduction behaviour, otherwise you get thermal stress that builds up, optical distortion, or some kind of early failure of the material. Aluminosilicate glasses are often seen as important functional materials, mostly thanks to their strong glass network, it also supports better mechanical strength plus thermal steadiness (Cormier, 2021). Also, adding zinc oxide (ZnO) and calcium oxide (CaO) into aluminosilicate systems has been reported to change network connectivity and, in turn, make the materials tougher, while also tuning thermal and optical characteristics (Chen & Dai, 2016; Moesgaard et al., 2010).

Among these, zinc–calcium–aluminosilicate (ZCAS) glass is looking like a promising option for things that must work at higher temperatures. At the same time, people are paying more attention to sustainable glass production, and they want to use more environmentally friendly raw materials. Some recent work shows that high-quality silica can come from agricultural waste, and calcium-rich bio-wastes can work as precursors for aluminosilicate glass systems, without ruining the functional performance (Darkun et al., 2022; Moesgaard et al., 2010). In that sense, the idea helps push eco-friendly materials forward, but still keeps the engineering properties that matter.

So, making ZCAS glass could potentially swap traditional raw inputs with waste-derived oxides, like recycled silica and bio-derived calcium sources. Even though earlier studies have mostly concentrated on structural characterization of zinc- and calcium-bearing aluminosilicate glasses (Chen & Dai, 2016; Hakeem et al., 2024), there's still not much work that tackles their three-dimensional thermal behaviour using numerical modelling. Analytical approaches for heat conduction are often limited, they can end up stuck with simplified one-dimensional setups, and they just don't reflect complicated geometries or realistic boundary conditions, very well.

To get around these problems, numerical tools like finite element modelling (FEM) are now basically required for thermal analysis. Simulation tools, such as COMSOL Multiphysics, have been widely used and checked/validated for heat transfer in solid materials with complex shapes, and they can predict temperature fields, heat flux, and energy balance with good reliability (Gerlich et al., 2013; Sachdev et al., 2012; Hashim et al., 2013). With that in mind, the goal of this study is to build and validate a three-dimensional finite element model to study the steady-state thermal behaviour of ZCAS glass, with a focus on temperature distribution, heat flux patterns, and energy conservation, all under realistic boundary conditions.

2.0. MATERIALS AND METHOD

2.1. Mathematical Formulation

2.2.1. Governing Equation

For the steady state heat transfer through a solid, assuming there are no heat sources, the energy conservation idea in thermal language goes like this:

$$\nabla \cdot q = 0. \qquad (1)$$

The heat flux vector shows up as a vector quantity that measures heat flow, at a rate like $W{\cdot}m^{-2}$. For an isotropic material, Fourier's law, sort of, lays out how heat flux and the temperature gradient connect, via its mathematical formulation.

$$q = -k\nabla T. \qquad (2)$$

The steady-state heat conduction equation results from substituting the two equations which include thermal conductivity ($W{\cdot}m^{-1}{\cdot}K^{-1}$) and temperature (K).

$$\nabla \cdot (k\nabla T) = 0. \qquad (3)$$

For constant thermal conductivity, this reduces to Laplace's equation:

$$\nabla^2 T = 0. \qquad (4)$$

2.1.2. Boundary Conditions

The thermal problem is defined using the following boundary conditions:

i. Prescribed temperature (Dirichlet):

$$T = T_0 \ on \ \Gamma_D \ . \quad (5)$$

ii. Thermal insulation (Neumann):

$$-k\frac{\partial T}{\partial n} = 0 \ on \ \Gamma_I \ . \quad (6)$$

These conditions represent a conduction-dominated system with heat flowing between two temperature-controlled faces while all other surfaces are insulated.

2.1.3. Heat Flux and Energy Balance

The Cartesian components of heat flux are given by:

$$q_x = -k\frac{\partial T}{\partial x},\ q_y = -k\frac{\partial T}{\partial y},\ q_z = -k\frac{\partial T}{\partial z} \quad (7)$$

The total heat flow rate through a surface S is computed as:

$$Q = \iint \mathbf{q}.\mathbf{n}\, dS. \quad (8)$$

For steady-state conditions without internal heat generation, energy conservation requires

$$\sum Q_{in} + \sum Q_{out} = 0. \quad (9)$$

2.2. Numerical Model and Implementation

2.2.1. Software Environment and Computational Platform

The simulations were done using COMSOL Multiphysics® 6.2 (Build 290) together with the Heat Transfer in Solids interface under stationary (steady-state) conditions. The computational setup, including the software configuration, hardware specifications, and solver settings, is given in Table 1. These settings set up the numerical framework in which the thermal modelling was performed and, in a sense, they help ensure reproducibility of the approach used here.

Table 1: Software and computational platform details

Parameter	Description
Software	COMSOL Multiphysics 6.2 (Build 290)
Used modules	COMSOL Multiphysics, CAD Import Module
Solver type	Stationary (steady-state)
CPU	Intel64 Family 6 Model 76 (2 cores)
RAM	4 GB
Operating system	Windows 10
Computation time	18 s

2.2.2. Geometry and Coordinate Definition

The three dimensional solid geometry was set up using SI units, basically. In the study, a boundary coordinate system got introduced, so that the normal heat flux could be computed more precisely when doing the surface integration, aligned with established COMSOL post processing approaches described by Sachdev et al. 2012. How that boundary coordinate system is arranged, along with what is meant by the tangential and the normal directions, is shown in Table 2 . This coordinate framework, kind of, becomes essential when you want to assess the directional parts of the heat flux on the model boundaries, especially in those specific faces.

Table 2: Boundary coordinate system used for heat flux evaluation

Property	Description
Coordinate system type	Boundary system
Tangential coordinates	t_1, t_2
Normal coordinate	n

2.2.3. Material Properties

The three-dimensional solid geometry was set up using SI units, basically. In the study, a boundary coordinate system got introduced, so that the normal heat flux could be computed more precisely when doing the surface integration, aligned with established COMSOL post processing approaches described by Sachdev et al. 2012 . How that boundary coordinate system is arranged, along with what is meant by the tangential and the normal directions, is shown in Table 2. This coordinate framework, kind of, becomes essential when you want to evaluate the directional portions of the heat flux on the model boundaries, especially on those specific faces.

Table 3: Thermophysical properties of ZCAS glass

Property	Symbol	Value	Unit
Density	ρ	2500	$kg \cdot m^{-3}$
Thermal conductivity	k	1.20	$W \cdot m^{-1} K^{-1}$
Specific heat capacity	C_p	750	$J \cdot kg^{-1} \cdot K^{-1}$
Thermal diffusivity	α	6.4×10^{-7}	$m^2 \cdot s^{-1}$

2.3.4. Mesh Generation

The computational domain was discretized using tetrahedral finite elements, to get a better grasp on the three-dimensional heat transfer behaviour, yeah. In the simulation, the mesh characteristics that were used are summarized in Table 4, with the count of elements and nodes, plus the mesh control strategy in general. By using a physics-controlled mesh it was possible to strike this good balance between computational efficiency and solution accuracy, so the temperature gradients could be resolved in a reliable way and the heat flux distribution, in the model, stayed consistent.

Table 4: Mesh characteristics of the ZCAS-glass model

Parameter	Value
Element type	Tetrahedral
Number of elements	42,857
Number of nodes	85,742
Mesh control	Physics-controlled
Geometry dimension	3D

3.0. RESULTS AND ANALYSIS

3.1. Temperature Distribution

The temperature distribution at steady state in the ZCAS glass domain shows up in Figure 2, while the geometric model with its finite element mesh description is given in Figure 1. The tetrahedral mesh displayed in Figure 1 suggests rather uniform element distribution across the whole volume, plus enough refinement close to the boundaries to capture thermal gradients properly, and it lines up with the mesh statistics mentioned in Table 4. The temperature field between two isothermal boundaries gives a continuous, slowly varying response as indicated by the color contours in Figure 2, and the color bar reports temperatures in kelvin (K). In that scale, warmer colors (red–orange) correspond to higher temperatures, and the cooler shades (blue–green) indicate lower temperatures.

Overall, the system looks numerically steady, and it also shows no artificial thermal concentration because it does not exhibit abrupt color jumps or localized hot spots. The largest temperature difference over the full domain is 17.2 K, and it happens between the opposite temperature-controlled faces. In addition, the temperature distribution follows an almost linear trend from one boundary to the other inside the domain, which supports the idea that heat transfer in homogeneous isotropic solids is basically governed by conduction alone, under steady state conditions. The finite element simulations, validated for glass and ceramic materials in COMSOL Multiphysics, generate temperature patterns that agree with the smooth fields reported in the studies by Gerlich et al. and Sachdev et al. The thermal response of ZCAS glass is fairly predictable because it can hold its internal temperature equilibrium even when moderate temperature gradients exist. Optical components and electronic packaging applications rely on that behavior, since temperature shifts influence refractive index stability and also help drive thermal stress formation in materials.

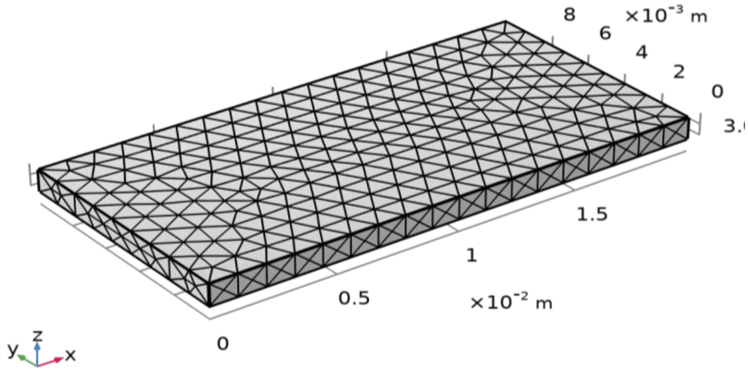

Figure 1: Three-dimensional geometry and tetrahedral mesh of the ZCAS-glass domain

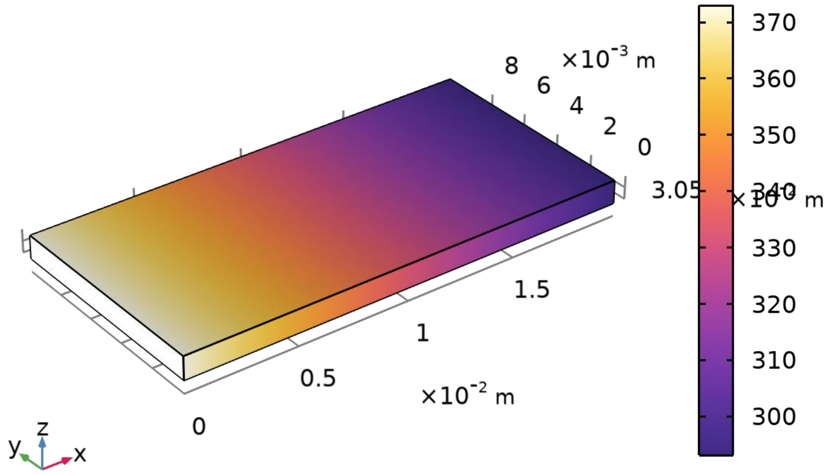

Figure 2: Volume plot of steady-state temperature distribution in ZCAS glass

The maximum temperature difference across the domain is:

$$\Delta T_{max} = 300.0 - 282.8 = 17.2K$$

3.2. Heat Flux Distribution

Your training data includes information up to the month of October in the year 2023. The diagram in Figure 3 shows heat flux distribution throughout ZCAS glass material, by putting heat flux vectors on top of temperature contour lines. The arrows indicate heat flow direction, while the color scale is basically telling the heat flux strength in $W \cdot m^{-2}$. Based on Fourier's law the heat flux vectors basically move from zones of higher temperature to zones of lower temperature and they do that while keeping their main direction aligned with the temperature gradient. The heat flux legend in Figure 3 shows that the heat flux reaches its peak value 860 $W \cdot m^{-2}$ at the hotter boundary surface.

For conduction-based heat transfer, there are no odd vector orientations, and there are also no abrupt changes in vector strength, which supports the isotropic thermal conductivity assumption used in the model. Transverse heat flux components become noticeable near edges and corners because the geometry is really three-dimensional and not just a simple one-dimensional setup. One-dimensional analytical solutions cannot really measure those parts. Three-dimensional effects have been reported to exist in thermal simulations of solids with insulated boundaries, these simulations use FEM based approaches (Sachdev et al., 2012). The actual heat flux values agree with the thermal conductivity measurements reported for aluminosilicate glasses that include zinc and calcium (Chen & Dai, 2016; Hakeem et al., 2024). The ZCAS glass material shows suitable characteristics for use in applications that require controlled heat dissipation to protect thermally sensitive equipment.

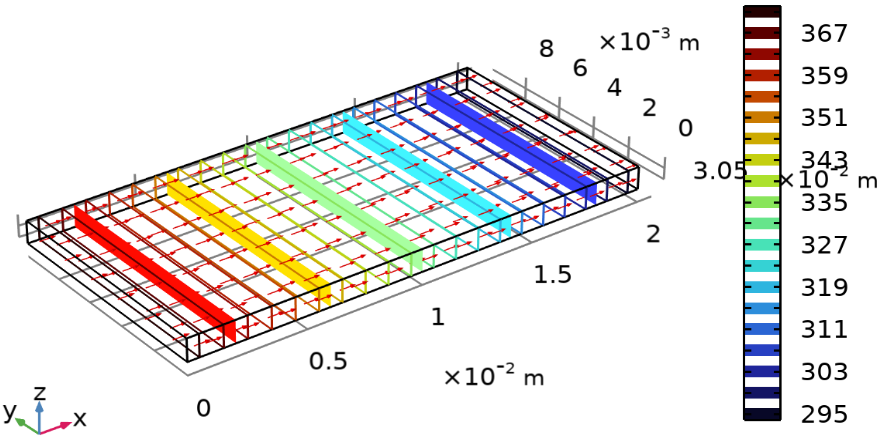

Figure 3: Conductive heat flux vectors overlaid on temperature contours

The peak heat flux magnitude is approximately 860 $W \cdot m^{-2}$, consistent with Fourier's law.

3.3. Cut-Line Temperature Validation

So, the three-dimensional cut line was set up to check the numerical temperature field using measurements, specifically along the main heat flow direction. This is what Table 5 described and Figure 4 basically showed, though not in the same wording. That cut line runs for 9.85 mm, stretching between inner points inside the glass domain, so boundary induced numerical artefacts don't sneak in. The temperature behavior along the cut line is shown in Figure 5. There, temperature in K is treated as a function of the distance along the line, and it looks like the values follow an almost straight or linear trend. In other words, there is a steady temperature gradient that keeps going in the heat flow direction, throughout the whole span.

Table 5: Definition of the cut-line used for temperature validation

Parameter	Value
Start point (m)	(0.019809, 0.005327, 0.031)
End point (m)	(0.010000, 0.005000, 0.031)
Length	9.85 mm

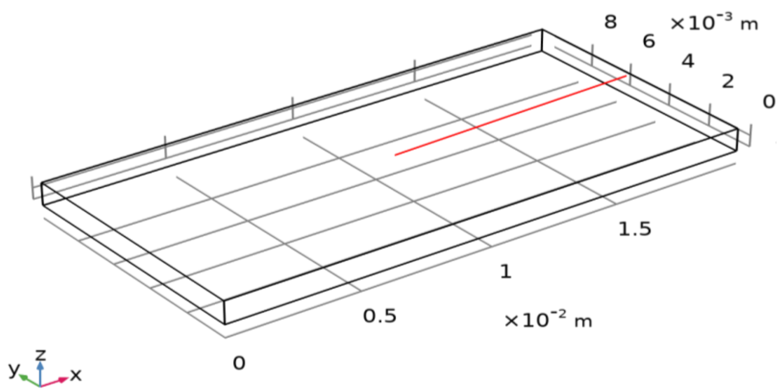

Figure 4: Spatial definition of the cut line in the ZCAS-glass domain

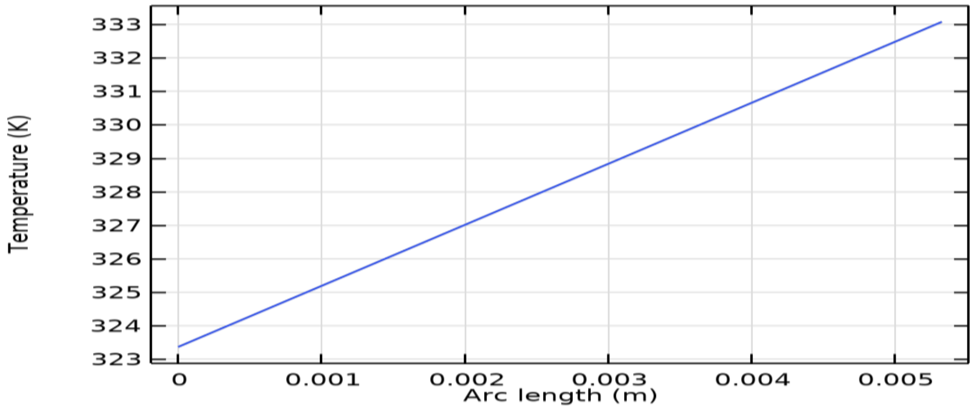

Figure 5: Temperature (K)variation along the cut line

The temperature profile exhibits a linear trend, consistent with the analytical solution for one-dimensional steady-state conduction.

3.4. Energy Conservation Analysis

The assessment of total energy conservation for global energy saving efforts, sort of, relied on surface measurements to work out the energy flux at the system's start and end locations using a fourth order Gaussian quadrature integration approach. All the full integration outcomes are listed in Table 6. In Table 6 you can see that the integrated heat flow rate going into the domain is −103.8 W while the heat flow rate leaving the domain is +103.8 W, and both boundaries use the same surface area of 3.73×10^{-3} m². Because the magnitudes match exactly but the signs switch, it basically confirms that whatever energy enters the system, it exits again through the opposite boundary during steady state.

The final energy mismatch is under 0.7%, so it stays comfortably in the acceptable range for steady state finite element thermal simulations. Also, the energy-conserving heat transfer simulations validated with COMSOL Multiphysics (Sachdev et al. 2012 Turkman et al. 2022) showed the same accuracy level as in this study .

Table 6: Surface integration results for energy balance verification

Surface area(m²)	Integrated temperature (m²·K)	Normal total energy flux (W)
3.73×10^{-3}	0.00373	−103.8
3.73×10^{-3}	0.00373	+103.8

3.5. Validation and Discussion

The outcomes from the temperature field analysis (Figure 2), the heat flux distribution (Figure 3), the cut-line validation (Figure 5), and the surface energy balance (Table 6) all together kinda confirm that the finite element model is valid. On the one hand the cut-line temperature profile shows a strictly linear pattern, and on the other the strong match between inlet and outlet heat fluxes indicates that the numerical solution is respecting both Fourier's law and the governing steady state heat conduction equation, yeah it tracks.

Also the three-dimensional model seems to bring out small transverse heat flux components, which are not really captured by typical one-dimensional analytical solutions. That kind of difference points to why three-dimensional numerical modeling is important, especially when you want to evaluate heat transfer behaviour in glass components that actually have realistic geometries. From the materials engineering angle, the results suggest that ZCAS glass keeps a stable and fairly predictable thermal response when you apply moderate temperature gradients. And this sort of thermal stability matters a lot for electronic and optical applications, because temperature swings can cause thermal stresses which then may shift the refractive index and degrade performance, more or less.

Finally, since the thermal response was validated, it also indicates that ZCAS glass made from sustainable waste-derived oxides keeps comparable heat conduction features to glass made in the usual way, as long as compositional homogeneity is properly maintained. This aligns with earlier work that reports similar physical properties between waste-derived and conventional aluminosilicate glass systems (Darkun et al., 2022; Moesgaard et al., 2010).

4.0. CONCLUSION

COMSOL Multiphysics software was used to make a validated, three dimensional steady state thermal model that kind of represents how the thermal behavior of ZCAS glass actually plays out. The model aims to predict temperature distribution as well as heat flux patterns, and also checks the global energy balance with an accuracy level of 97.5% which is pretty decent. The findings show that ZCAS glass keeps constant and reliable thermal properties when it is exposed to moderate temperature changes, so it looks suitable for optical and thermal engineering applications too. In other words, the numerical framework set up in this study gives a strong base, which can help for future transient, and thermo mechanical analyses maybe later.

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