

Modeling Reaction-Diffusion Systems in Affinity-based Biomaterials for Tissue Engineering

Hydrogels are widely used as protein delivery vehicles. Modeling protein release and retention profiles may help bioengineers optimize their drug delivery strategies for regenerative medicine applications.

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Introduction

Hydrogels are water-swollen polymer matrices with mechanical properties similar to soft tissues. As such, bioengineers have leveraged these constructs to expedite tissue repair, often loading them with cells, small molecule drugs, and proteins. Proteins are of particular interest as their presentation can enhance cell recruitment and proliferation, guide specialized differentiation, and modulate overall tissue behavior. However, proteins freely loaded into hydrogels may suffer from rapid burst release upon implantation.

Controlled release of protein drugs is necessary to prolong protein bioactivity and reduce off-target side effects. The Hettiaratchi lab specializes in the design of affibodies, small protein scaffolds that selectively and reversibly bind to a given protein. The bioconjugation of affibodies to hydrogel matrices allows for tunable control over the spatiotemporal presentation of proteins. Our model seeks to elucidate the effect of these affinity interactions on the release and retention of a variety of proteins.

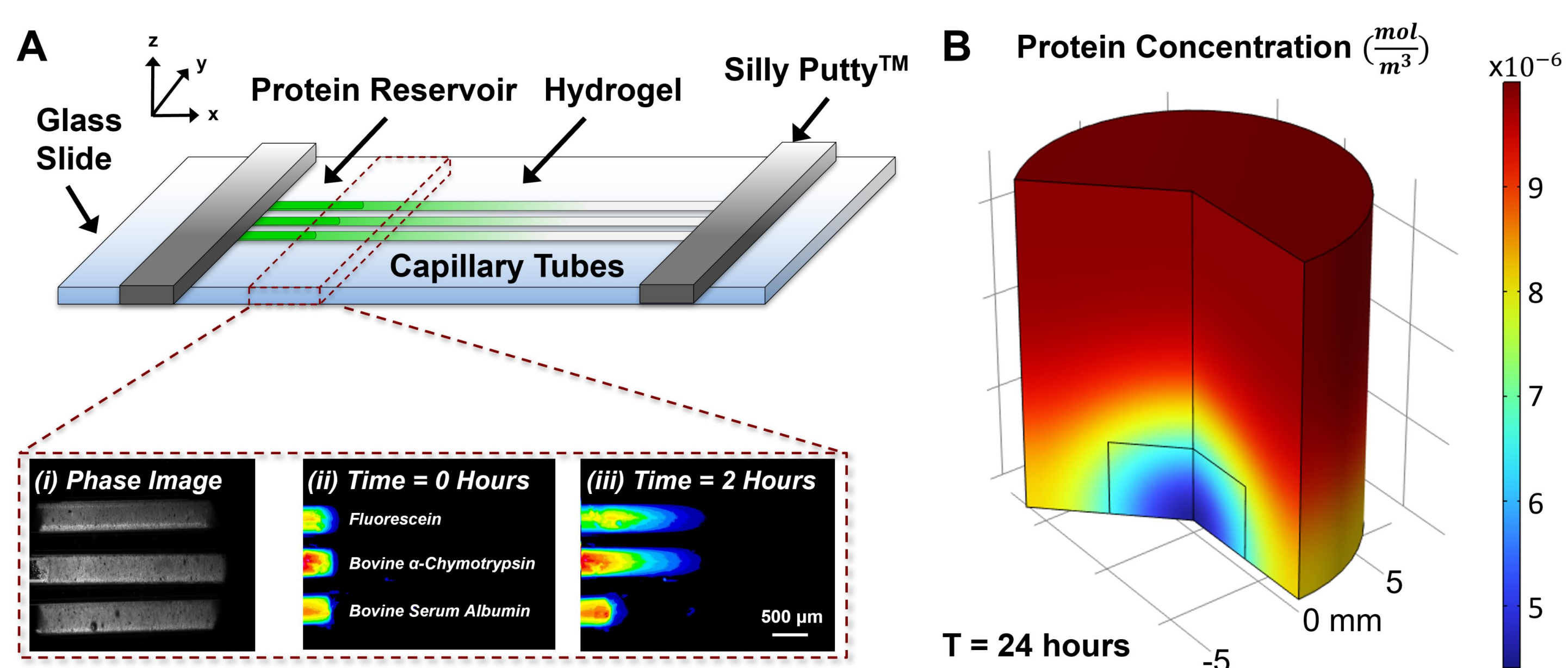


FIGURE 1. A: *In vitro* capillary system used to validate model of protein diffusion in hydrogels. B: Affibody-coupled hydrogels sequestering protein from a concentrated solution.

Methodology

Protein diffusion through hydrogel matrices was evaluated *in vitro* using a capillary tube setup. Fluorescence intensity from molecularly tagged proteins was used to describe protein diffusion using Eq1. This system was then modeled using the Transport of Dilute Species Physics module.¹ A 4x8 mm hydrogel in a 24-well plate was then modeled to evaluate protein sequestration by affibody-coupled hydrogels using Eq2.

$$\text{Equation 1. } F(x, t) \propto \operatorname{erfc}\left(\frac{x}{2\sqrt{D_{eff}t}}\right)$$

$$\text{Equation 2. } K_D = \frac{[\text{Protein}] * [\text{Affibody}]}{[\text{Affibody-Protein Complex}]} = 1.07 * 10^{-5} \left(\frac{\text{mol}}{\text{m}^3}\right) = \frac{k_{off}}{k_{on}}$$

Results

No significant difference in protein diffusion was found between *in vitro* and *in silico* capillary tube models.¹ This work from the lab provides a rapid method for determining protein diffusion coefficients in hydrogel formulations. Figure 2 showcases the steady-state behavior of affibody-protein complexes within our model of a hydrogel in a 24-well plate. Here, the ratio of steady-state concentrations for unbound proteins and affibody-protein complexes approximates to an equilibrium dissociation constant of $1.07 * 10^{-5} \left(\frac{\text{mol}}{\text{m}^3}\right)$. The strength of the affinity interactions between the affibody and target protein can be altered to tune the final release/retention profile. Future work will look to couple the effect of a hydrogel's porosity with varying affinity strength of our affibodies to determine the diffusivity of target proteins.

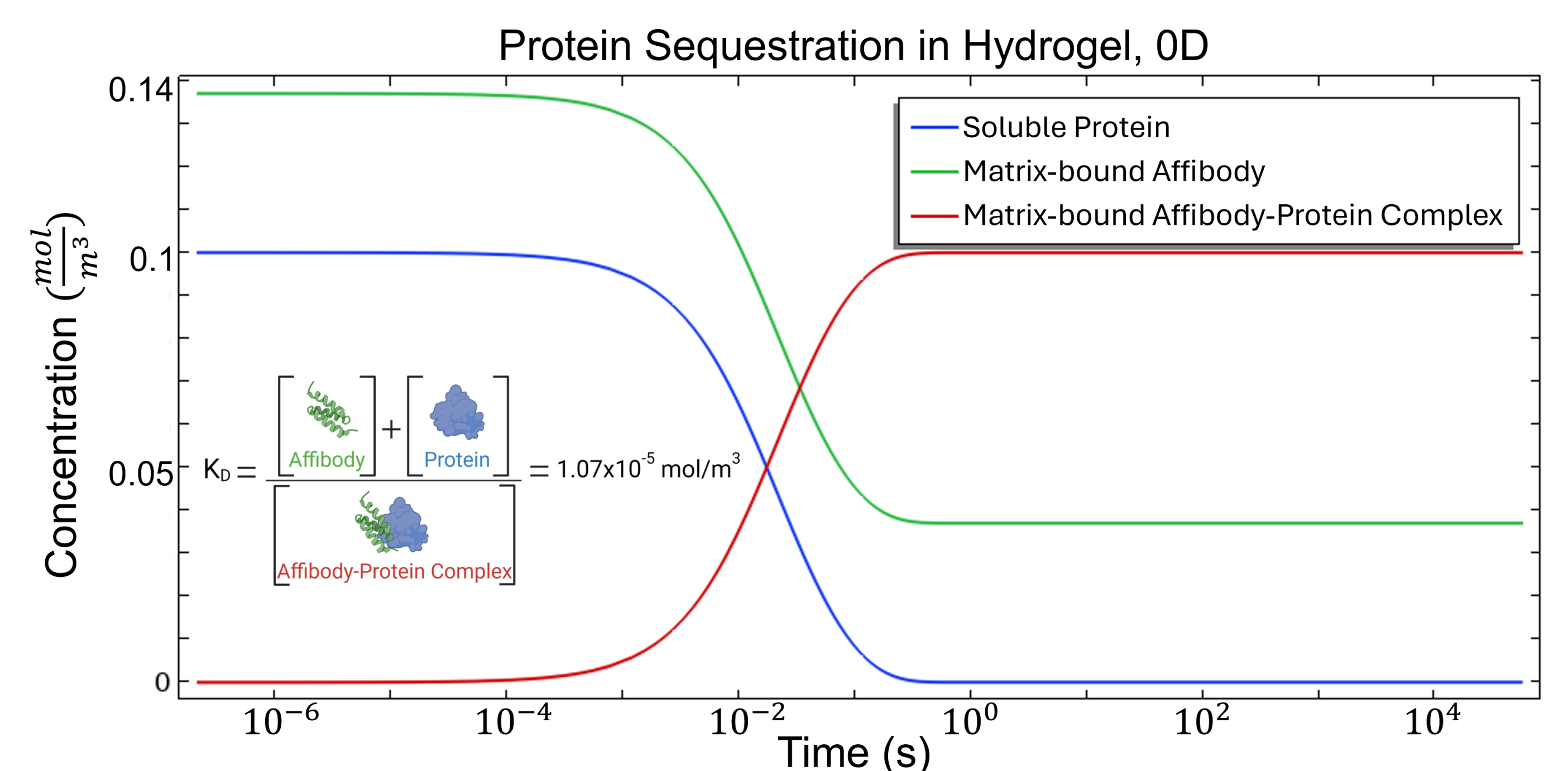


FIGURE 2. Steady-state behavior of affibodies, soluble protein, and affibody-protein complexes. K_D values used for the system are from high affinity affibodies previously developed by the lab.²

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1. M. Hettiaratchi, "A rapid method for determining protein diffusion through hydrogels for regenerative medicine applications", *APL Bioeng.*, vol. 2, pp. 026110, 2018.
2. J. Dorogin, "Moderate-Affinity Affibodies Modulate the Delivery and Bioactivity of Bone Morphogenetic Protein-2", *Adv. Healthc. Mater.*, vol. 12, pp. 2300793, 2023.



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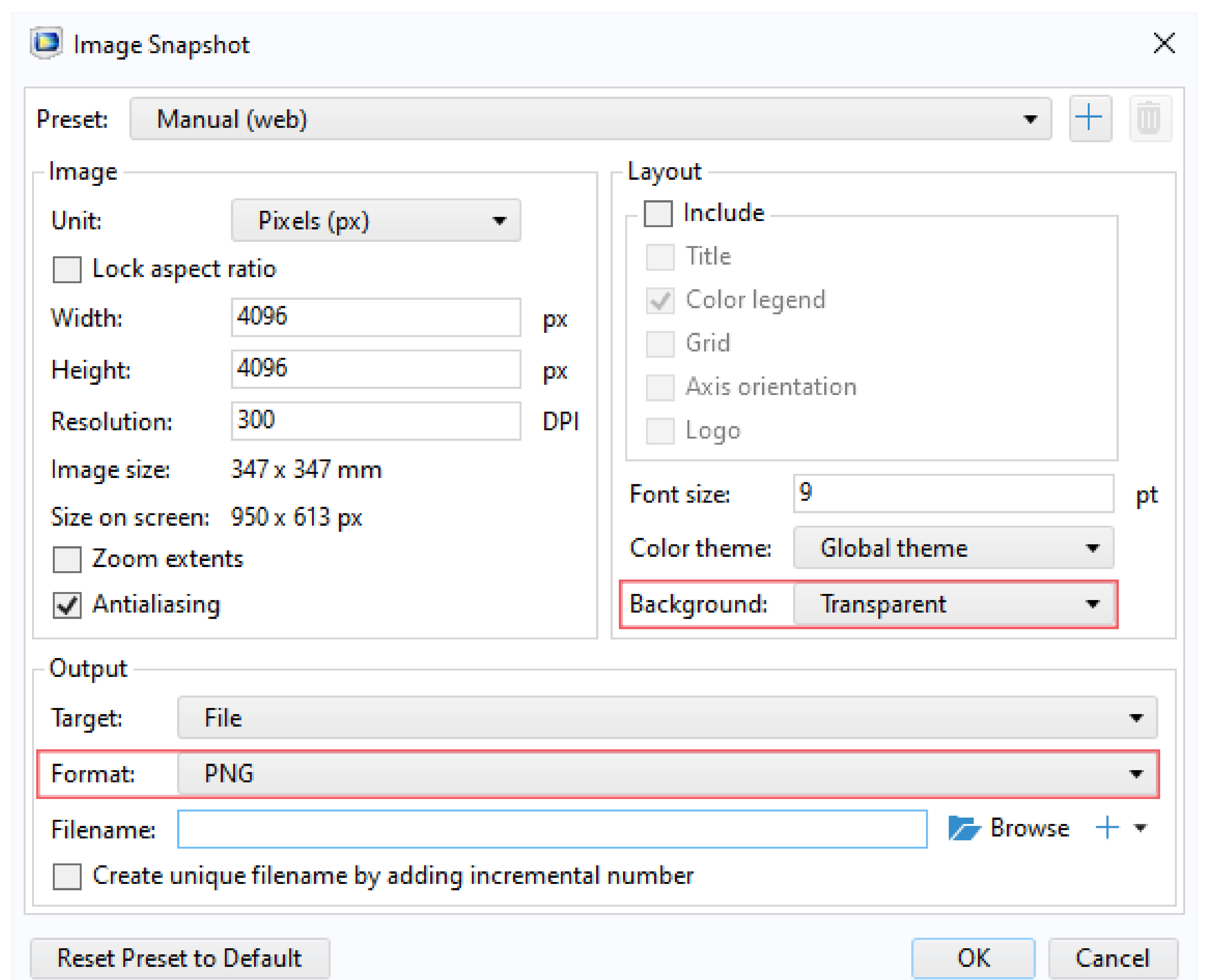
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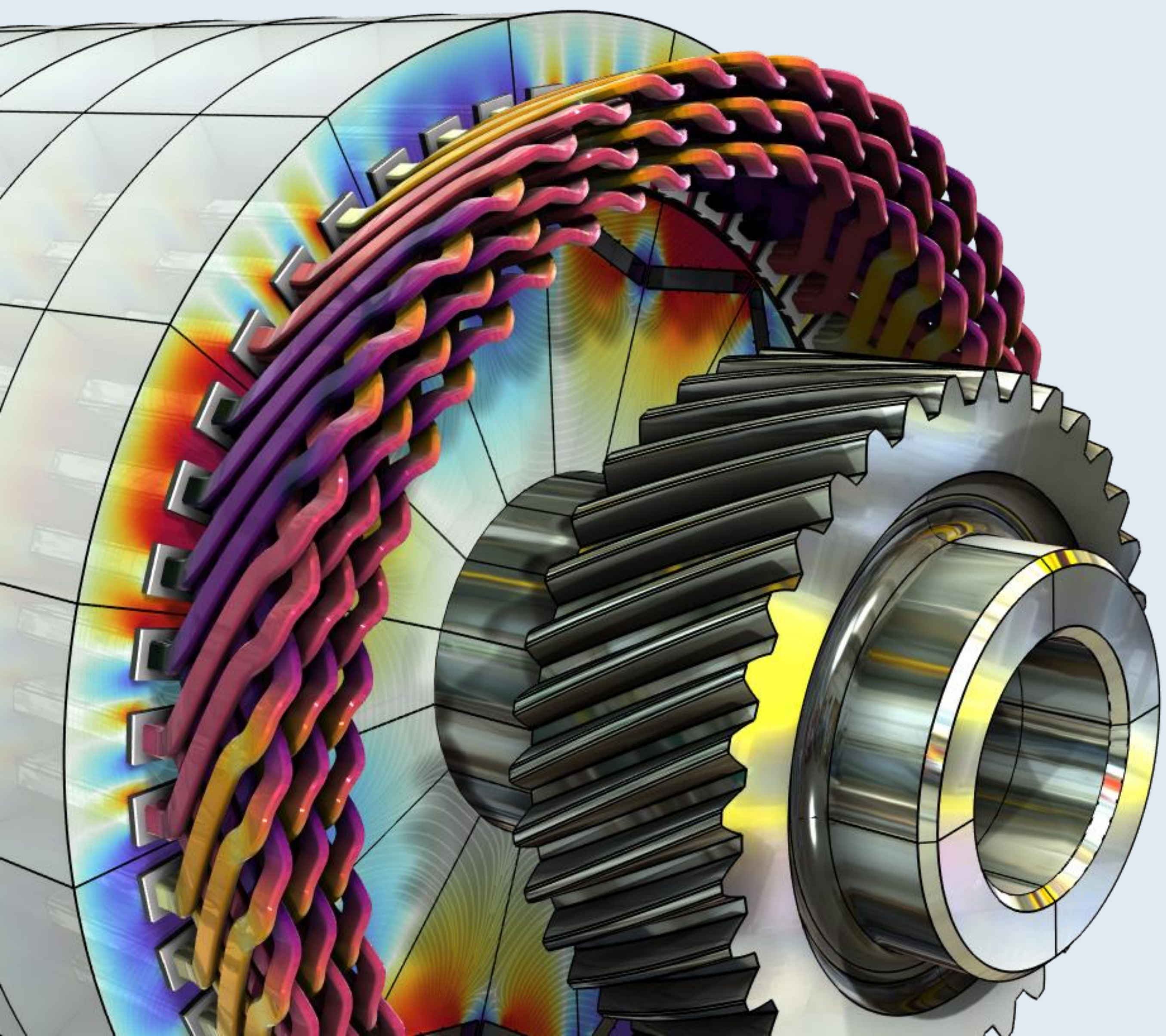
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Analysis of a Permanent Magnet Motor in 3D

Optimize permanent magnet (PM) motor performance by understanding their full behavior, including sensitivity to high temperatures.

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Abstract

While PM motors are valued for the energy savings that they provide, there are some design limitations to address. For example, permanent magnets are sensitive to high temperatures. Such temperatures can occur when currents, particularly eddy currents, generate heat losses.

The findings offer greater insight into the behavior of PM motors, particularly by capturing the eddy current losses that occur within the magnets. This information serves as a useful resource for improving the design of PM motors, and therefore the technology they help power.

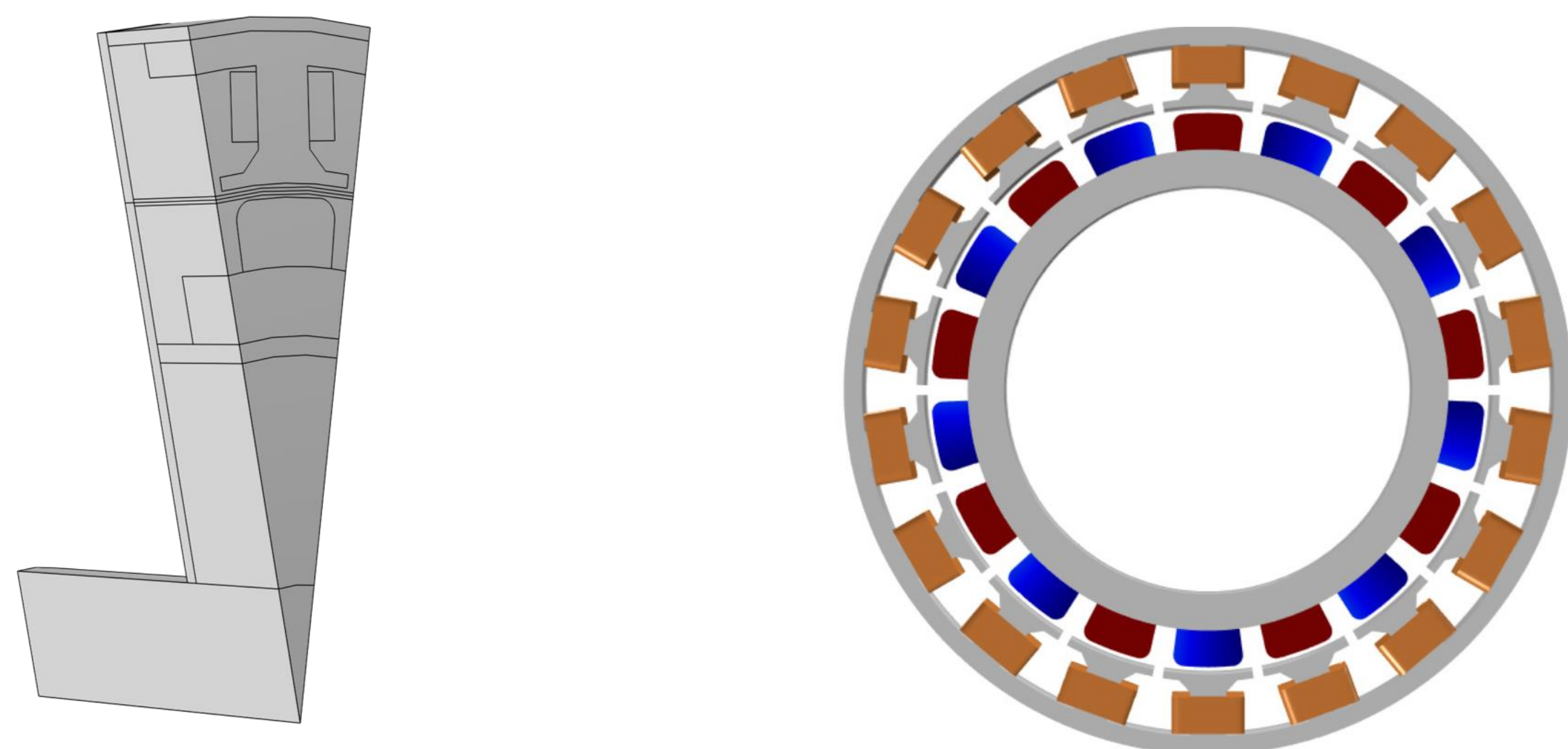


FIGURE 1. Left: Permanent motor sector. Right: Drawing of the PM motor.

Methodology

An 18-pole PM motor is modeled in 3D. Sector symmetry and axial mirror symmetry are utilized to reduce the computational effort while capturing the full 3D behavior of the device.

The conducting part of the rotor is modeled using Ampère's law:

$$\sigma \frac{\delta \mathbf{A}}{\delta t} + \nabla \times \left(\frac{1}{\mu} \nabla \times \mathbf{A} \right) = 0$$

Results

The results can be seen in Figure 2, which shows the magnetic flux density for the motor in its stationary state, that is, the initial conditions for the time-dependent simulation. In this state, the coil current is zero. It also shows the magnetic flux density for the motor after revolving one sector angle. In this plot, the air and coil domains are excluded in order to get a better view.

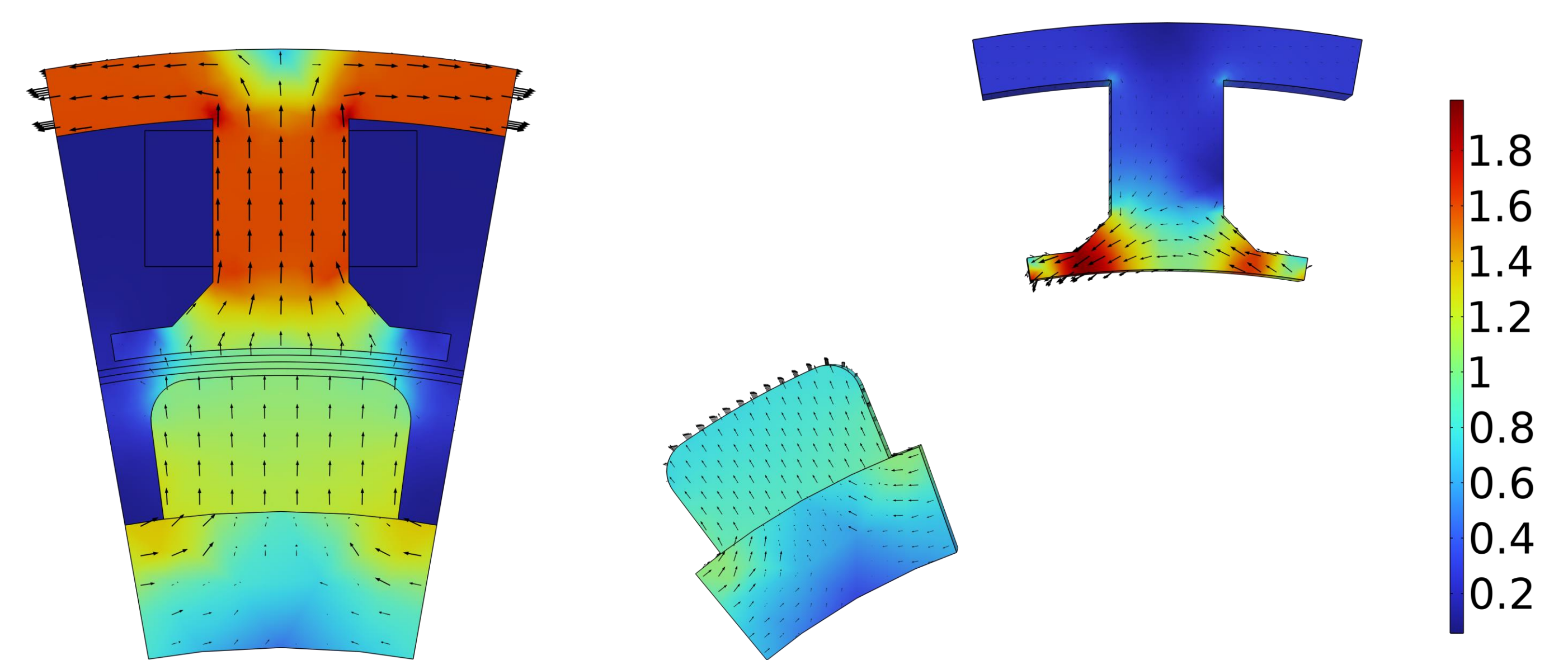
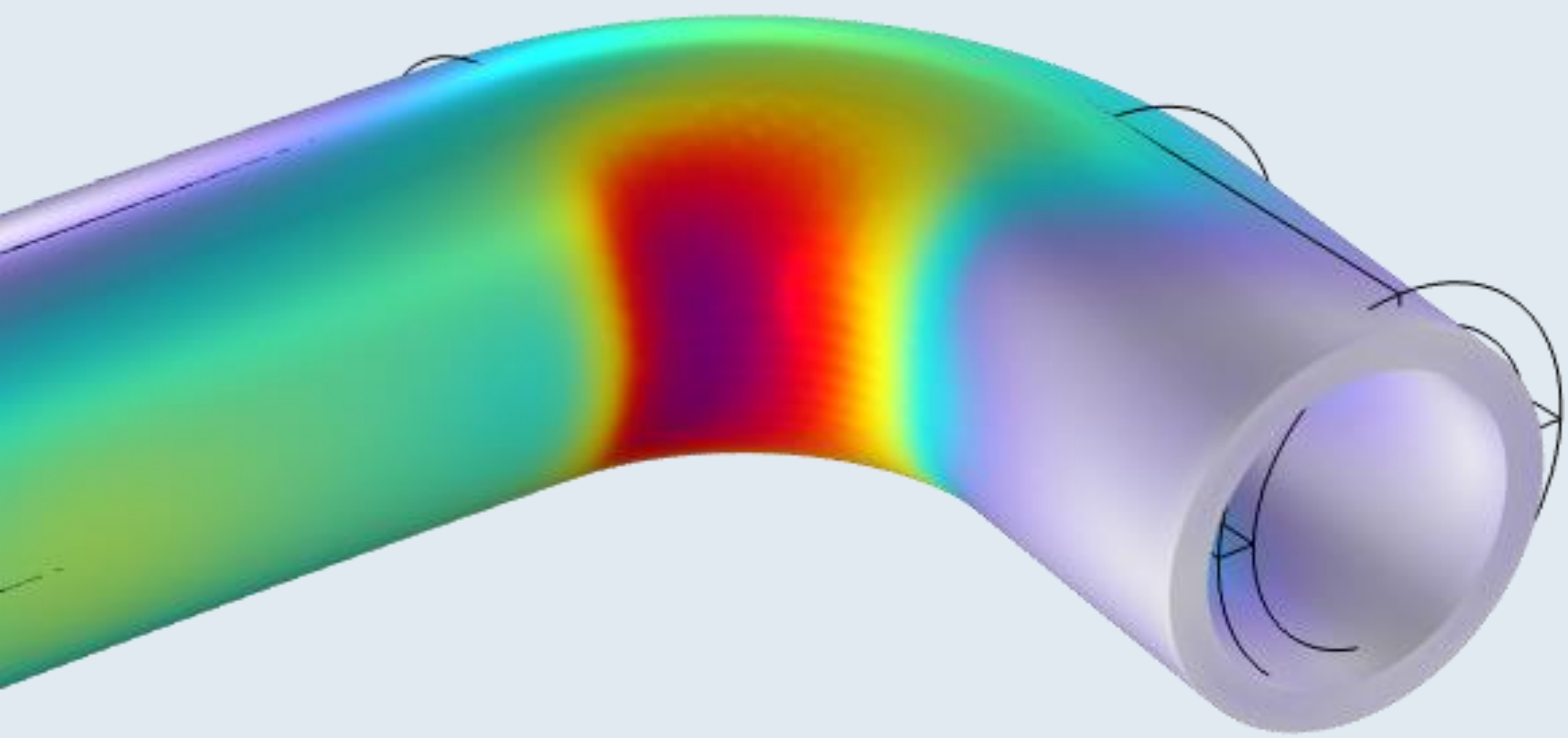


FIGURE 2. Left: Magnetic flux density from the permanent magnets with only the rotor at rest. Right: Magnetic flux density after revolving one sector angle.

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3. Author first initial and last name, "Article Title", *Journal*, Volume (vol.), Page numbers (pp.), Year.



The Intriguing Stresses in Pipe Bends

For many structural engineers, beam theory is a popular analysis tool. Using the equations can be beneficial when considering structural behavior, as they are easy to apply and provide useful results. This work investigates one such case.

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Introduction & Goals

Pipe bends are common in piping systems, which typically transport liquids or gas, often under high pressure. One place where you may find a lot of pipes are oil tankers. The labyrinthine piping systems can look pretty fascinating.

Many piping standards (or codes) used for industrial applications are based on beam theory when it comes to the structural analysis. But, as we have already discovered, pipe bends generally do not

behave like beams. When digging into piping standards, you will find a lot of information dedicated to pipe bends. In particular, piping standards recommend to apply correction factors to the stiffness and stresses for curved pipe sections. (Ref. 1)



FIGURE 1. Piping systems on an oil/chemical tanker. Image licensed under CC BY-SA 3.0 via Wikimedia Commons.

Methodology

The pipe is slender with a constant cross section, so it would seem like a natural choice to treat such a structure as a beam in a simplified analysis. The bending moment is the only load acting on the structure, and it's thus constant for any given section along the entire beam axis.

The maximum stress even occurs on the *inside* of the pipe. The cross section of the bend also deforms significantly, and, more specifically, it ovalizes with the major axis either being oriented in the bend plane or perpendicular to it depending on the direction of the bending moment.

Results

At a relative thickness of $t/R_0 \approx 35\%$ (which for any real application would be considered very thick), the stress distribution starts to change quite significantly. Additional perpendicular tensional stresses superpose the beam solution at the inner- and outer-bend radii.

Simultaneously, the top and bottom of the pipe show compressional stresses. These additional circumferential stresses arise due to the ovalization of the cross section. Ordinary beam theory explicitly ignores such cross-sectional deformations, and it does fall short in capturing its effect.

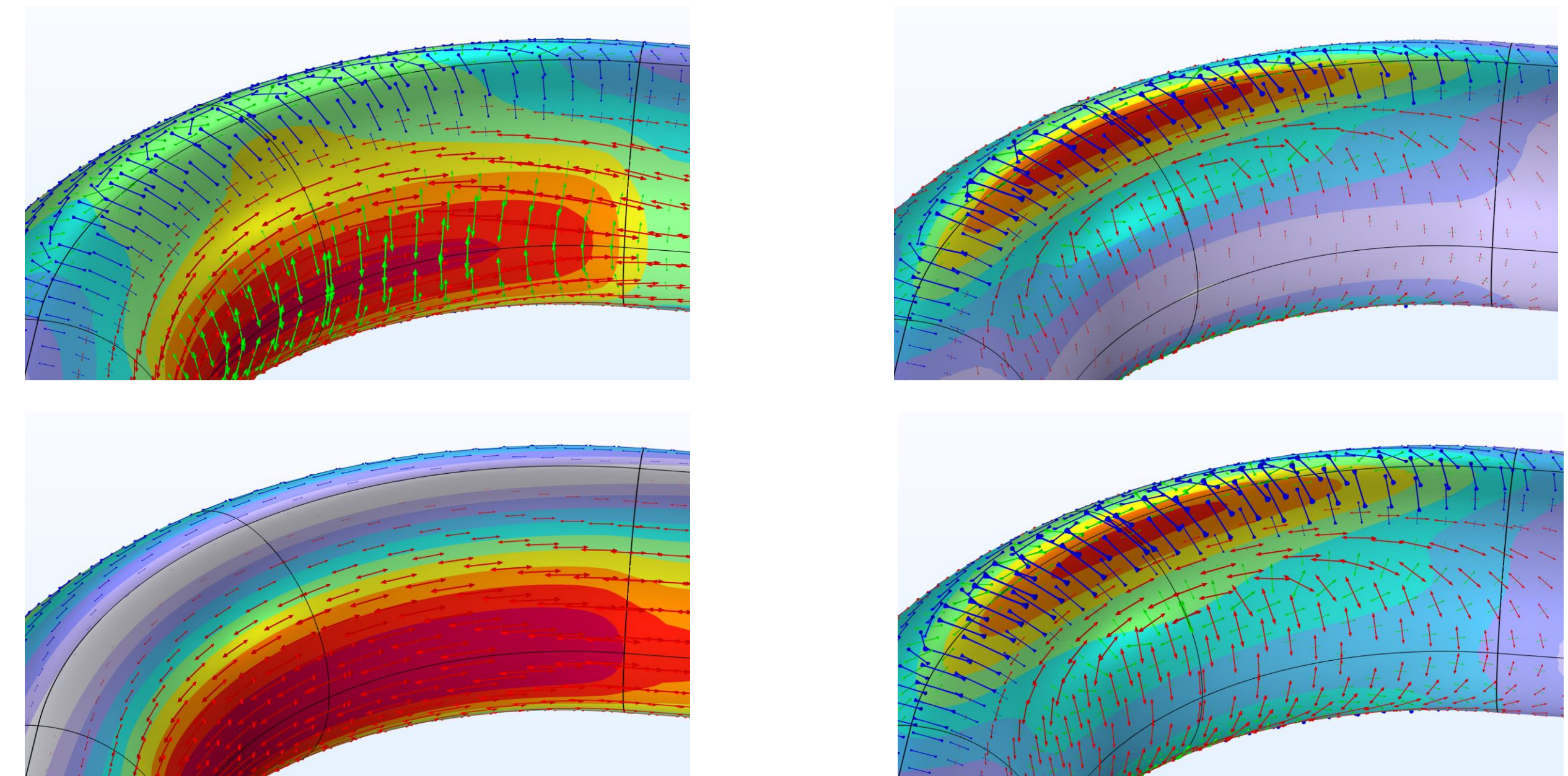


FIGURE 2. View of the pipe bend showing the von Mises stress (normalized) and principal stresses for different wall thicknesses.

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1. E.A. Wais and E.C. Rodabaugh, "Background of SIFs and Stress Indices for Moment Loadings of Piping Components", United States, 2005; <https://www.osti.gov/biblio/841246>
2. "Stress Intensification Factors (i-Factors), Flexibility Factors (k-Factors), and Their Determination for Metallic Piping Components", ASME, 2017; <https://www.asme.org/codes-standards/find-codes-standards/b31j-stress-intensification-factors-flexibility-factors-determination-metallic-piping-components/2017/drm-enabled-pdf>