CENIDE & WIN Seminar Series on 2D-MATURE

DFG IRTG 2803 & NSERC CREATE

Nickolas Eaves

University of Windsor

"Modeling of gas-phase formation of carbonaceous nanomaterials"

March 27th, 2025
10:00 a.m. ET / 16:00 p.m. CET

Dr. Eaves expertise is in nanomaterial formation in chemically reacting high-temperature flows with a focus on numerical model development. Dr. Eaves co-authored two detailed numerical codes, CoFlame and PRESS, that have been published and are freely available to the research community. These research codes represent the state of the art in carbon black formation modeling, including fluid dynamics, chemical kinetics, thermodynamics, radiation, and particle dynamics. He has worked on developing fundamental physics-based models for the least understood part of carbon black formation, which is the birth of particles or inception. His works in this area represented a ground-breaking advancement towards the development of predictive carbon black formation models. In recent years, he has turned his attention to developing models for other high-value carbon nanomaterials such as graphene, and investigating co-generation of hydrogen and nanomaterials from fossil fuels towards a net-zero CO2 economy.

Carbon-based nanomaterials formed in the gas phase exhibit a range of properties, with some being beneficial and others harmful. In combustion processes within the energy and transportation sectors, spherical carbon nanoparticles, commonly known as soot, are significant contributors to climate change and are linked to cancer. Conversely, carbon black and graphene, produced in controlled, specialized reactors, offer substantial advantages. Carbon black is similar to soot; however, it is one of the highest-volume and highest-value nanomaterials globally. Graphene is a Nobel Prize-winning 2D planar material that is renowned for its exceptional properties. These materials all originate from the formation of large molecules called polycyclic aromatic hydrocarbons (PAHs) in the gas phase. This research talk centers on developing and applying fundamental models to understand the behavior of these PAHs and the conditions that favor the formation of either spherical particles like soot and carbon black, or planar 2D materials like graphene. The numerical code CoFlame, a custom FORTRAN chemically reacting CFD code, is the main tool used in the research.