## Clarkson University Department of Chemical and Biomolecular Engineering SEMINAR

Ruan de Villiers (Ph.D. Candidate, Clarkson University) will speak on:

## Parallel column model for Reactive Dividing Wall Column simulation

As part of the ongoing optimization of chemical production processes, process intensification has yielded concepts such as reactive distillation and the dividing wall column. In recent years, modelling of reactive dividing wall columns (RDWCs), the combination of these two technologies, has attracted significant attention because simulations of processes containing such columns have demonstrated the potential for significant savings in terms of both energy expenditure and capital cost. Most modelling of these columns requires decomposing RDWCs into a thermodynamically equivalent flowsheet of reactive and non-reactive column sections in a sequential modular process simulation package. Such simulations of (R)DWCs can be time consuming to create and difficult to converge. It has been suggested that equation-oriented solvers can have superior numerical performance. This presentation will demonstrate the results of development of a CAPE-OPEN compliant equation-based parallel column model (PCM) that enables the rapid modelling of an RDWC as a single self-contained unit operation. Some conventionally modelled RDWCs from the literature are reproduced with the PCM to demonstrate its validity and excellent numerical performance. The ease of use and rapidity with which different RDWC configurations can be created is a significant advantage of our PCM.

## Monday, September 12<sup>th</sup>, 2022 at 3:00 pm Science Center 344



Ruan de Villiers holds a BS in Chemical Engineering from the University of Texas at Austin. He is currently a Ph.D. candidate in the department of Chemical and Biomolecular Engineering at Clarkson University working with Prof. Ross Taylor.