

Abstract Submitted
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Kinetics of Vascular Remodeling: Comparison of Solver Approaches R.C. WARD, ORNL, J.J. NUTARO, ORNL, K.L. KRUSE, ORNL, E.C. O'QUINN, A.R. REEDY-JACKSON, M.M. WOERNER — Results will be presented for kinetics of matrix metalloproteinases (MMP), enzymes that play a significant role in vascular remodeling. Three different computational approaches for well-mixed kinetics processes will be analyzed and compared. The kinetics of one MMP, namely MMP2, were elucidated using a model and rate constants from published literature¹ and implemented using the *JSim* environment (see nsr.bioeng.washington.edu). Further investigations of this pathway were undertaken using System Biology Workbench (SBW) (see sbw.kgi.edu), where the system of kinetic equations was created using an interactive visual interface. Using SBW the complexity of the kinetics was evaluated using phase space analysis. Finally, we implemented the kinetics model using Discrete Event System Specification (DEVS). Using *adev* (see www.ece.arizona.edu/~nutaro), an open-source DEVS modeling environment we demonstrate that continuous, well-mixed, enzyme kinetics can be modeled using discrete event simulation. The three computational environments will be compared and their utility and comprehensiveness evaluated. 1. Karagiannis, E. D. and Popel, A. S., J. of Biological Chemistry, **279** (37):39105–39114, 2004.

Richard Ward
ORNL

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