

# Correlations in Chemical Reaction Kinetics

PI: Uwe C. Täuber, Virginia Tech, DMR-0308548

## Research:

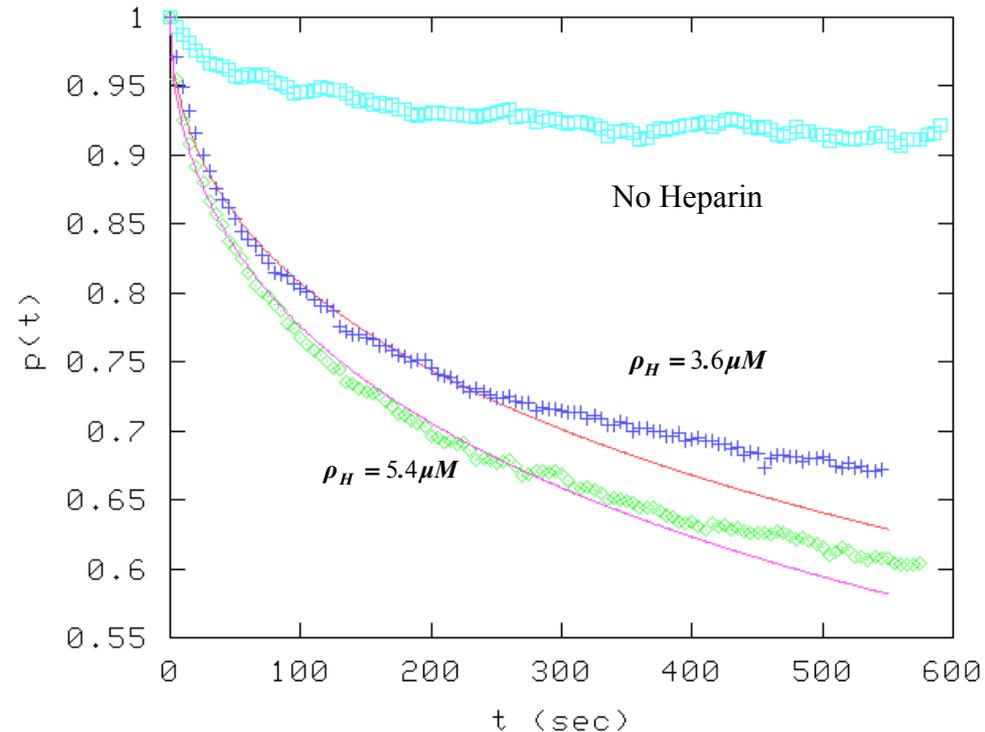
Signal transduction into the interior of cells via transmembrane receptor proteins is initiated by binding of specific ligands (e.g., growth factors).

In collaboration with **Kim Forsten-Williams** (Chemical Engineering, Virginia Tech) and postdoctoral associate **Manoj Gopalakrishnan**, we have studied the effects of (possibly multiple) ligand rebinding on the dissociation curve.

We devised a self-consistent approach to determine the fraction of bound ligands  $p(t)$  as function of time. We compared our results with both computer simulations and experimental data obtained in vitro for insulin-like growth factor (IGFBP-3) by means of the surface plasmon resonance (SPR) technique. We find strong deviations from the exponential predicted by the standard rate equation approach: Multiple rebinding leads to considerably slower dissociation.

Such effects are especially prominent when the ligands are not uniformly distributed on the cell membrane, but clustered into “lipid rafts”.

[M. Gopalakroshnan et al., e-prints q-bio.QM/0406004 and q-bio.SC/0407015.]



*Figure:* IGFBP-3 dissociation curves as obtained by SPR in the presence and absence of rebinding-suppressing heparin (concentrations as indicated). Notice the markedly non-exponential decay in the absence of heparin. The lines represent theoretical curves from our self-consistent mean-field theory, appropriately fitted to the experimental data.

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## Education:

This interdisciplinary project involved graduate students **Theresa R. Cassino** and **Luz Padro** (both in Chemical Engineering), **Satheesh Angaiah** (Electrical and Computer Engineering), and undergraduate student **Eric Spiegel** (Physics).

**Eric Spiegel** graduated in spring 2004 and then entered the graduate program in physics at Virginia Tech.

**Manoj Gopalakrishnan** moved on to a postdoctoral position in theoretical biophysics in Frank Jülicher's group at the Max Planck Institute for the Physics of Complex Systems at Dresden, Germany.

In another research project, physics undergraduate student **Mark. J. Washenberger** undertook a crucial role in devising and running a versatile Monte Carlo simulation code for the study of various diffusion-limited reactions.

Specifically, in collaboration with **Henk J. Hilhorst** (Université Paris-Sud Orsay, France) and former postdoctoral associate **Olivier Deloubrière**, we investigated the temporal decay laws for several variants of diffusion-limited multi-species pair annihilation processes.

[*H.J. Hilhorst et al., J. Phys. A: Math. Gen.* **37**, 7063 (2004) and e-print cond-mat/0409079.]