

Modelling the Vulcanization Reaction of Devulcanized Rubber

UNIVERSITY OF
WATERLOO

uwaterloo.ca

Ankita Saikia

Supervisor: Prof. Costas Tzoganakis

Background

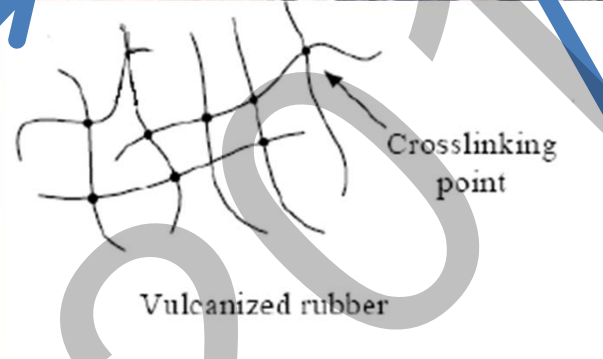
Virgin / Raw Rubber



Vulcanization/
Crosslinking

Vulcanized rubber

Is it same
or
different???



Pollution/
Health &
Fire Hazards

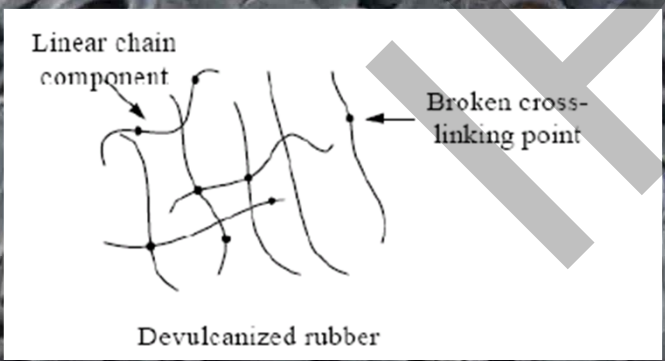
End life

Need to characterize the
vulcanization reaction!!!

Devulcanized Rubber

Devulcanization

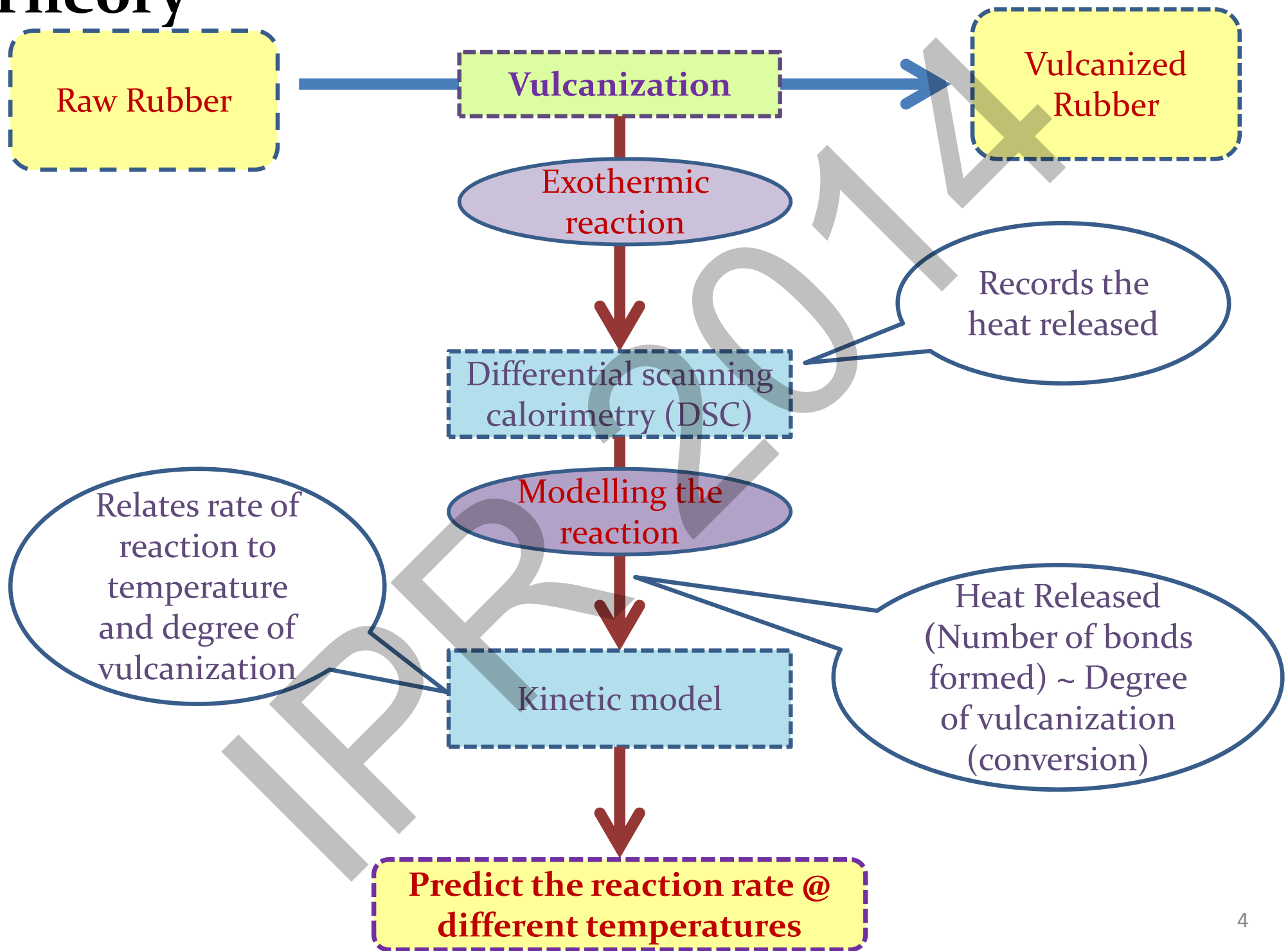
Scrap
tires/rubber



Objectives

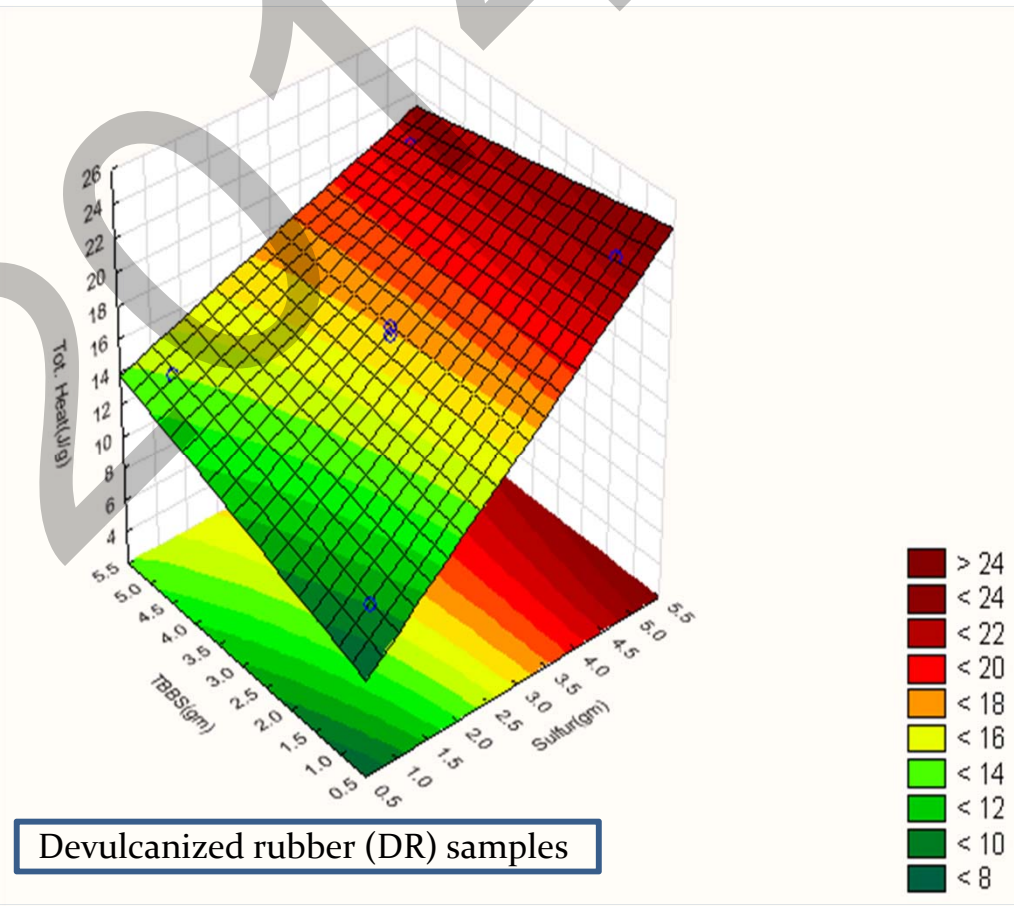
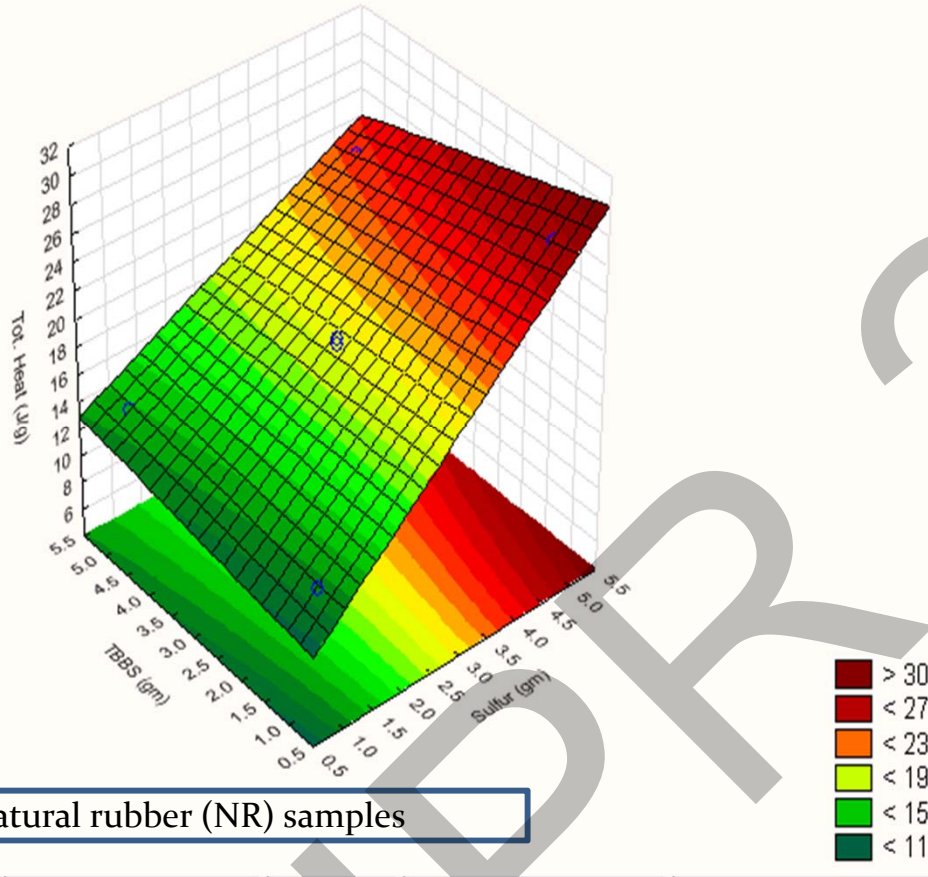
- To study the vulcanization reaction of devulcanized rubber by differential scanning calorimetry (DSC).
- To model the vulcanization behavior of devulcanized rubber.
- To compare the vulcanization behavior of virgin rubber and devulcanized rubber.

Theory

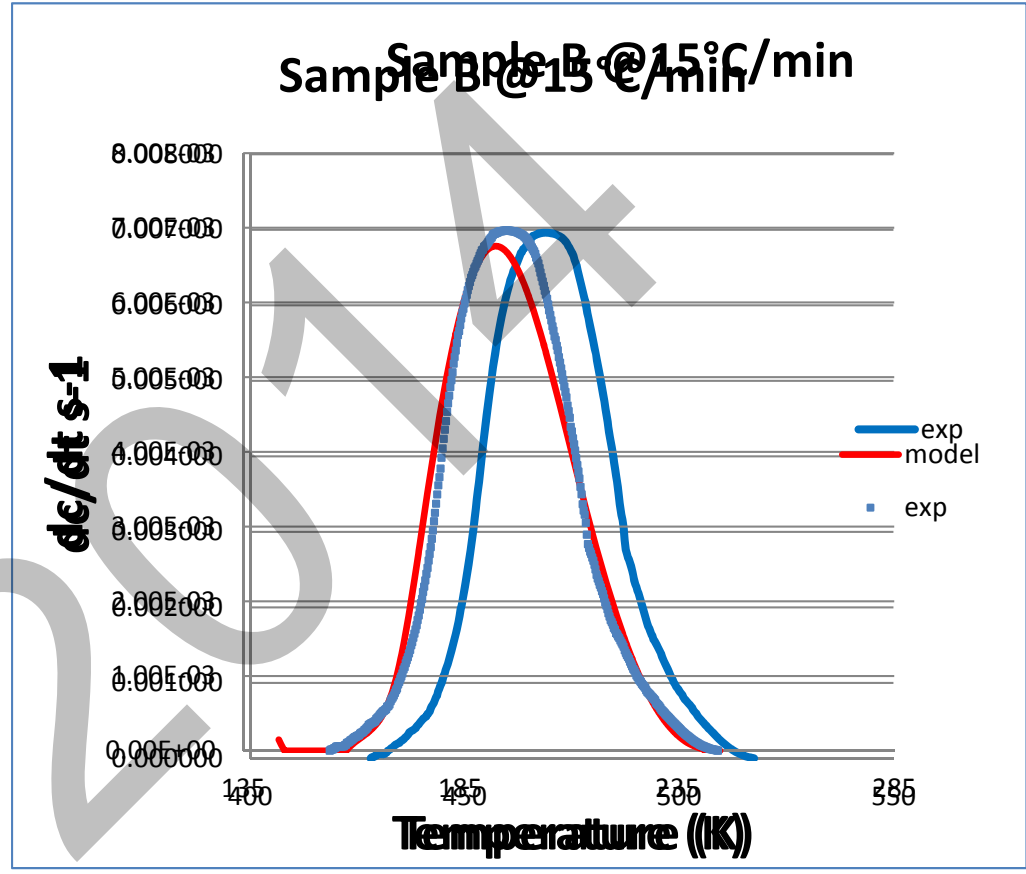
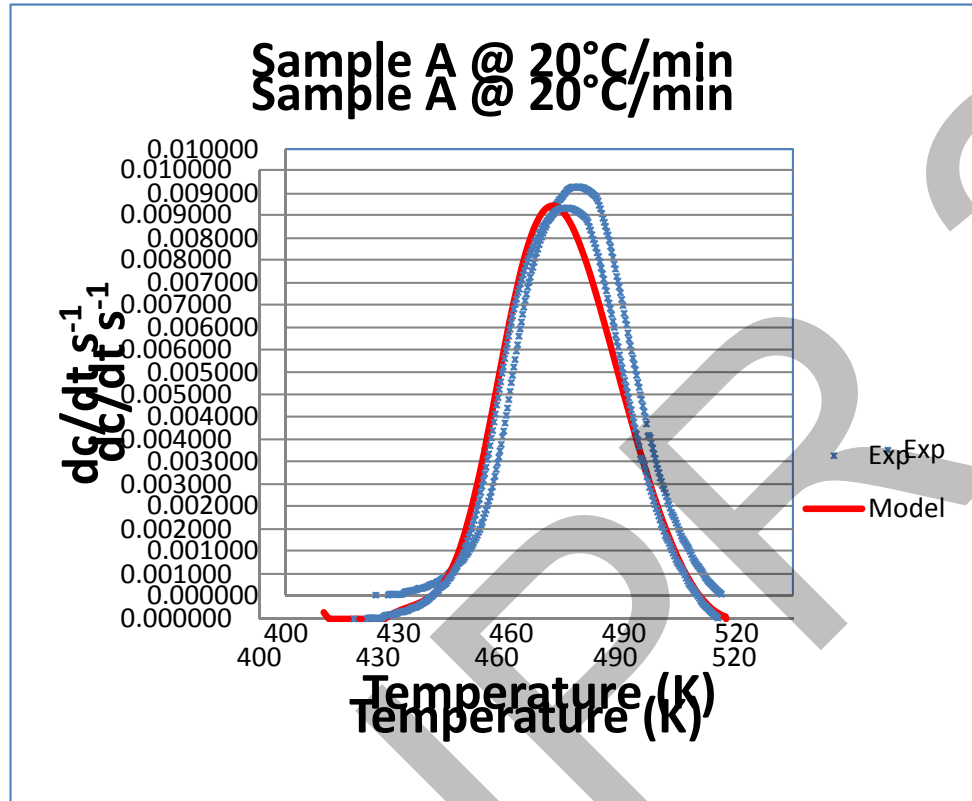


Results

- Effect of change in curative composition in total heat of reaction



➤ Fitted model and experimental data for natural rubber sample at different scan rates.



Summary

- The vulcanization enthalpy (heat of reaction) is seen to be linearly proportional to the initial sulfur content.
- The total heat of reaction follows the similar trend for both natural and devulcanized rubber .
- The fitted models are in good agreement with the experimental data , the constants obtained can be used to predict reaction rate and degree of vulcanization at different temperatures.

**Thank you!!
Questions??**

➤ Approaches to characterize a vulcanization reaction :

- Mechanistic model
- **Phenomenological model**

Kissinger Model

$$dc/dt = k(1-c)^n$$

dc/dt = rate of reaction
 k = rate constant
 c = degree of vulcanization
 n = order of reaction

Arrhenius Model $k(T) = a \exp(-E/RT)$

a = frequency factor
 E = activation energy
 T = Temperature
 R = Universal gas constant

Activation Energy

Kamal-Sourour Model

$$dc/dt = (k_1 + k_2 * c^m) * (1-c)^n$$

m and n are order of reaction.

6 parameters in the model (i.e. a_1, a_2, E_1, E_2, m and n) can be fit to experimental DSC data via least squares estimation algorithm.

References:

- Lopez, L. M.; Cosgrove, A. B.; Hernandez-Ortiz, J. P.; Osswald, T. A. Polym Eng Sci 2007, 47, 675–683.
- Musa R. Kamal, Polym Eng Sci 1974, 14, 231-239

