EXECUTIVE SUMMARY

The goal of the investigation was to be able to establish a delivery system for Thiobacillus ferrooxidans inhibitors that would be active for three to five years on coal mine dumps.

Initial work was centered around the use of rubber pellets. These pellets were the newest delivery system available in the USA. They were extruded by B.F.Goodridge and superceded the rubber sheet technique. These sheets were buried under the ground at various intervals in the mine dumps surfaces and in the state of Pennsylvania gave very favourable inhibition results.

The work centered around two facets. One to improve the pellet release device and secondly to minimize the amount of rubber matrix used by forming sachet devices. (Concentrated solution of inhibitor held in a sachet where the walls are slow release membranes.)

The work proved the following:

1. Monolithic elastomeric pellets containing various loadings of dissolved/dispersed SLS can be prepared satisfactorily.

2. Novel membrane devices, which release SLS at constant rates, can be prepared and the use of such devices for the long-term inhibition of the bacterial oxidation of pyrite in mine dumps give such promising laboratory results as to warrant protection being sought.

3. It is possible to determine the solubility limits of SLS in the various elastomers by means of differential scanning calorimetry (DSC), which show that phase separation occurs when the solubility limit of SLS in a particular rubber is exceeded. The onset of phase separation is characterized by an endotherm that appeared at 115°C. The solubility limits of SLS in the different elastomers vary. The solubility limits of SLS in natural rubber and in synthetic polyisoprene are 4% and 3%, respectively, when formulations are stored at °C before analysis. Storage of the natural-rubber formulations at room temperature for six months causes the solubility limit of SLS to increase to 9%.

4. High loadings of SLS in the various elastomers interfere seriously with the vulcanization process. The Borchardt & Daniels DSC Kinetics Data Analysis software, used to study the effects of the SLS loadings on the vulcanization of elastomers, can be used to analyze curing exotherms.

5. Mathematical models, given in the literature, give poor correlation between experimental data and theoretically-predicted values, which indicates that the release of SLS does not follow $t^{1/2}$ order kinetics.

6. Investigation of the effects of various factors on the rate of release of SLS from monolithic elastomeric pellets shows the following:

   6.1 The initial SLS loading in elastomeric pellets affects the release rate dramatically, but the relationship between the release rate and the SLS loading is non-linear. Loadings of up to 25% SLS have very little effect on the release rate, whereas loadings of 35% and more cause a dramatic increase in the release rate. This indicates that a second mechanism of release operates at SLS loadings of 35%

and more. This mechanism is postulated and to be the result of the creation of pores in the elastomeric matrices.

6.2 The addition of release promotors ($CaCO_3$ and $(NH_4)_2SO_4$) has virtually no effect on the rate of release of SLS from the particular formulations.

6.3 The pH of the eluent affects the release rate, especially when the matrices contain $CaCO_3$, but the effect is not significant enough to outweigh the effects of the other variables.

6.4 The base elastomer (NR, SBR, NR/SBR blend or IR) influences the release rate of SLS, with the release rates being the highest from the elastomer which displays the greatest solvation power for SLS.

6.5 **The most effective method for attaining a desirable rate of release of SLS is by varying the surface area to volume ratios of elastomeric pellets.**

7. An existing mathematical model to determine the effective diffusion coefficients of SLS in natural and synthetic rubbers gives a poor fit to the experimental data, probably due to the invalidity of the assumption that diffusion coefficients are independent of SLS concentration.

8. The values of the diffusion coefficients depend on the SLS loadings in the elastomeric pellets. It is suggested that the amount of porosity created in elastomeric pellets is a function of the SLS loading, and the concept of a concentration-dependent diffusion coefficient supports the argument for the dependence of the release rate on porosity.

9. A new model has been developed, based on a numerical method commonly used for predicting processes such as heat transfer and fluid flow. This model, which incorporates the effect of porosity development on the rate of release of SLS by employing a concentration-dependent diffusion coefficient, can be used as the basis of further investigation of the relationship between the diffusion coefficient and the concentration of SLS in rubber pellets.

10. An iterative procedure, which involves the use of the tri-diagonal matrix algorithm (Thomas algorithm), can be used to predict numerically the rate of release of SLS from cylindrical pellets. This procedure can be implemented by a FORTRAN program written for the purpose.

11. When it was assumed that the relationship between the diffusion coefficient and the concentration of SLS in the pellet is as follows:

$$\text{For } C > C_\alpha \qquad D = D_0$$

$$\text{For } C \leq C_\alpha \qquad D = (D_1 - D_0)\left(\frac{C_\alpha - C}{C_\alpha - 0}\right)^1 + D_0$$

$$= (C_K * D_0 - D_0)\left(\frac{C_\alpha - C}{C_\alpha}\right) + D_0$$

where $D_1 = C_K D_0$, a much-improved correlation between experimentally-determined and theoretically-predicted data could be obtained for elastomeric pellets containing 35% to 55% SLS.

12. The research findings on monolithic elastomeric pellets have been used by the Chamber of Mines in investigations on simulated coal dumps at the Wolwekrans mine near Witbank, Transvaal.

13. The release of SLS, from a saturated reservoir, through membranes containing no SLS, as well as through those containing 10% SLS, follows zero-order kinetics. It is apparent that when the membranes contain 35% SLS, two release mechanisms are involved. Membranes containing 35% SLS initially appear to function as monolithic devices, but during the last half of the test period the release rate is constant.

14. The high steady-state release rates obtained with elastomeric membranes containing 35% SLS strongly support the theory of a leakage flow, such as would be caused by porosity. Scanning electron microscopy studies on cross-section of leached NR/35% SLS membranes indicate that the membranes were porous. The studies on elastomeric membranes confirm the dependence of the release rate of SLS on the type of rubber used.

15. Contrary to generalized findings in the literature, the flux of SLS does not vary significantly with membrane thickness. The presence of a surface phenomenon (boundary-layer effect), occuring as the result of the micellar structure of SLS molecules, is proposed to explain these findings.

16. **The elastomeric membrane sachet reservoir is the most economic use of carrier (rubber) the time scale of release is predictable and can be extended to a number of years.**

17. **The reservoir release devices can also be used in inhibiting corrosion in mine cooling water where there is a need to inhibit Thiobacillus ferrooxidans.**

18. **The program has been fully successful in the creation of a useable dosing system for inhibitor, namely the sachet.**