# TOMSK POLYTECHNIC UNIVERSITY

## INFLUENCE OF FLOW RATE OF LINEAR ALKYLBENZENE IN FILM SULFONATION REACTOR ON CONCENTRATION OF TARGET PRODUCT AND TETRALINES AND SULFONES CONCENTRATION

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#### **RESEARCH OBJECT**

Linear alkilbenzenesulphonated (LABS) represent chemicals with a saturated hydrocarbonic chain from 10–13 atoms of carbon connected with one or sulfonate groups. These substances are one of the widespread anions used for production of synthetic detergents. Raw materials for production of LABS is an alkilbenzenesulphuric acid (ASA) which is produced as a result of course of the following stages: 1) dehydrogenation of alkanes with receiving an alkenes on Pt-catalyst; 2) benzene alkylation by olefins with production linear alkylbenzene (LAB). 3) sulphonation of LAB in a film reactor.

#### **RESULTS AND DISCUSSION**

The SO<sub>3</sub>/LAB molar ratio determines the medium acidity and finally the concentration of the viscosity components (the sulfones formation accelerates with the growth of the medium acidity). We use the SO<sub>3</sub>/LAB molar ratio as this is one of the most important and measured technological parameters. From the illustrative results given below we can see how the optimal conditions depend on the content of aromatics in the feed flow and amount of accumulated high viscosity components; see Fig. 2 and Tab. 2.

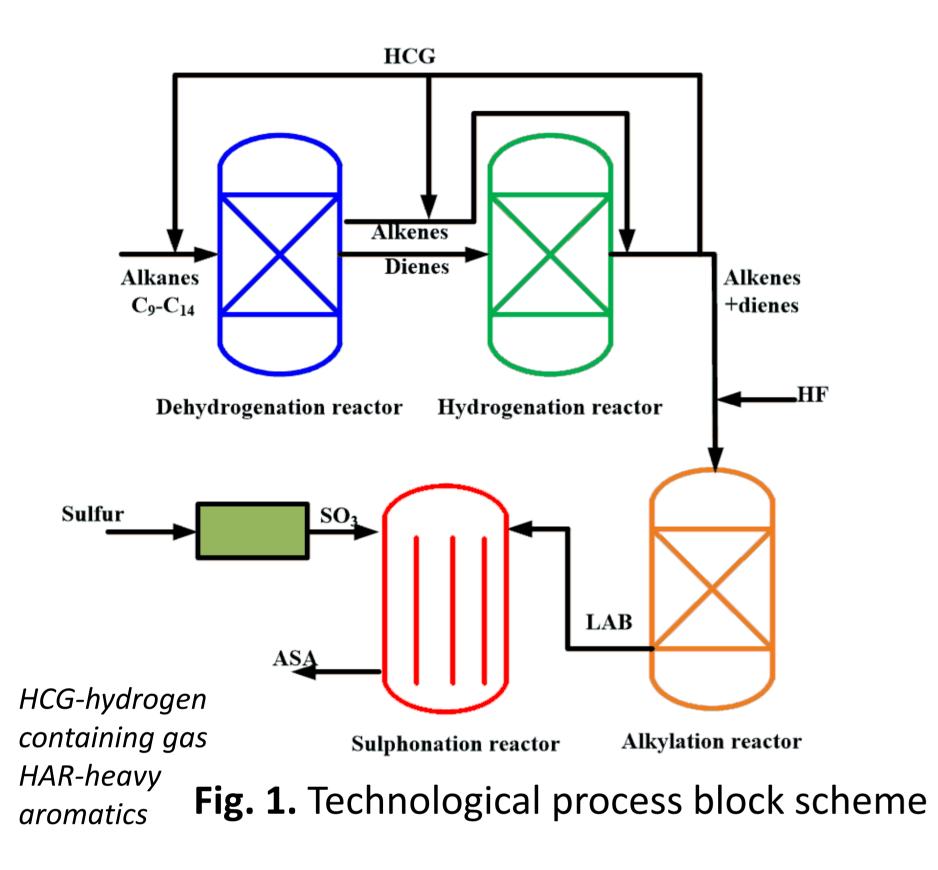
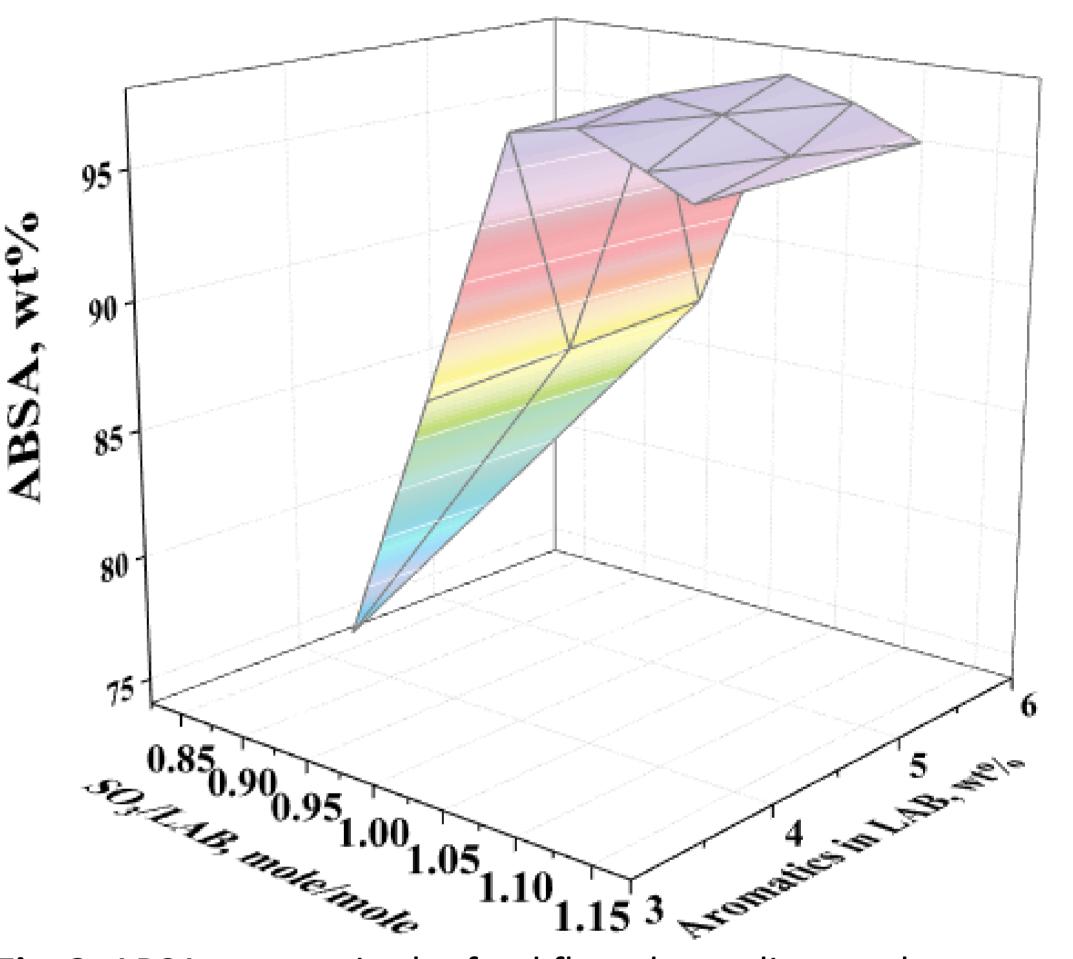


Table 1. Characteristics of sulphonation product and feed flows

Characteristics of the feed		Characteristics of the product			
flow		flow			
LAB content in	96-98	Active matter	≥ 96		
the feed flow,		content, wt.%			
wt.%					
LAB bromine	3-5	Unsulfonated	≤ 2		
index,		matter content,			
mg/100g.		wt.%			
2-	≥ 15	H <sub>2</sub> SO <sub>4</sub> content,	≤ 2		
phenylalkanes		<b>wt.%</b>			
in LAB, wt.%					
Linear isomer	≥ 93	ABSA color,	≥ 80		
in LAB, wt.%		Klett units			
SO <sub>3</sub> /LAB molar	0.98-1.05	ABSA viscosity,	≤ 175		
ratio, mole-		cSt			
mole					

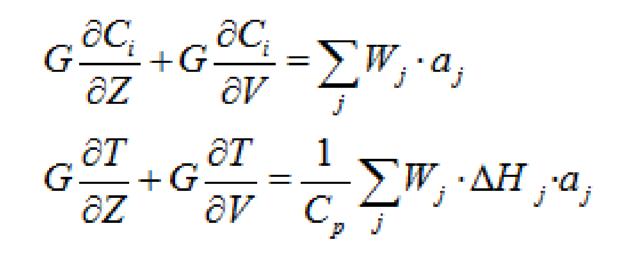
The purpose of present work was to show how  $SO_3/LAB$  molar ratio in the sulfonation reactor influences the



sulfonation process performance.

### **RESEARCH METHODS**

The research was performed using the computer modeling system of LAB sulfonation process.



 $Z=0, C_i=C_i^{in}, T=T^{in};$ 

 $V=0, C_i=C_i^{in}, T=T^{in}.$ 

Here the activity of reaction mixture is defined as:  $a_j = e^{-\alpha_j C_{v.c.}}$ , If Z=0 C<sub>v.c.=</sub>0, a=1.

Here  $a_{j}$  change in the rate of *j*-th reaction with the viscous component accumulation;  $C_{v.c.}$  concentration of high viscous component, mole/l; G – flow rate of raw materials, kg/h;  $W_j$  – rate of the *j*-th reaction, mole/(m<sup>3</sup>·sec);  $\Delta H_j$  – heat effect of the *j*-th reaction, K; T – temperature, K;

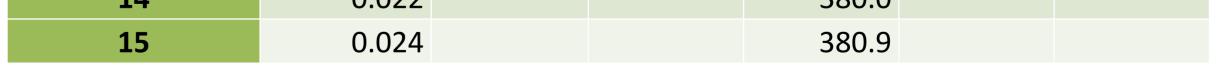
**Fig. 2.** ABSA content in the feed flow depending on the amount of accumulated high viscosity component and aromatics content in the feed flow.

Table 2. Effect of optimal  $SO_3/LAB$  molar ratio maintaining (model calculations)

Day of the period	<b>Concentration of the accumulated</b>			<b>Optimal sulfur flow rate to be</b>		
between reactor	high viscosity component, wt.%			converted to SO <sub>3</sub> , kg/h		
washings	Feed 1	Feed 2	Feed 3	Feed 1	Feed 2	Feed 3
1	0.003	0.004	0.005	371.7	371.8	372.1
2	0.005	0.006	0.007	372.2	372.5	372.8
3	0.007	0.008	0.01	372.8	373.2	373.6
4	0.008	0.01	0.012	373.4	373.9	374.4
5	0.010	0.012	0.014	373.9	374.7	375.2
6	0.011	0.014	0.016	374.5	375.4	376
7	0.013	0.015	0.018	375.1	376.2	376.8
8	0.014	0.017	0.02	375.8	377	377.8
9	0.016	0.019	0.021	376.4	377.9	378.8
10	0.017	0.021	0.023	377.1	378.8	380.1
11	0.018	0.022		377.7	379.7	
12	0.020	0.024		378.5	380.8	
13	0.021			379.2		
14	0.022			380.0		

 $T^{in}$  – initial temperature, K;  $C^{in}$  – initial concentration, mole/l.

The concentration of high viscosity components is calculated via mathematical model. If the current concentration is less the critical value, we fix this concentration as the initial value and repeat calculations using the same feedstock composition and technological modes. The critical concentration of the highly viscous component is the signal to stop the forecasting calculations. The number of such calculation cycles is the number of days between reactor washings.



The amount of sulfur to be converted into SO3 grows along with accumulation of high viscosity component between the reactor washings. This balances the reaction rates and keeps the ASA content in the product flow at minimum required constant level (96 wt.%). It is noticeable that for the feed flow 3 with high content of undesirable alkylaromatics the optimal amount of sulfur is the highest, in contrast to number of days between reactor washings.

