



The Russian Federation
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Nanotechnology and Biotechnology Department
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The Modeling of Gasoline Permeation through New Polymeric Materials

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NNSTU – the best traditions of Soviet and Russian engineering school



GAZ – Russian producer of LCV



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- **Introduction**
- **Theoretical background**
- **Modeling**
- **Mathematical model verification**
- **Conclusion**



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Metal vs Plastic... Why?



**Driven by the need to reduce weight
and improve fuel efficiency!**

INTRODUCTION



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	Advantages	Disadvantages
Metal	High temperature resistance Solidity	Price Corrosion Conductive Weight
Plastic	Price Low corrosion Lighter weight Vibration/sound damping Easily forming	Soft UV-corrosion



Fuel tank

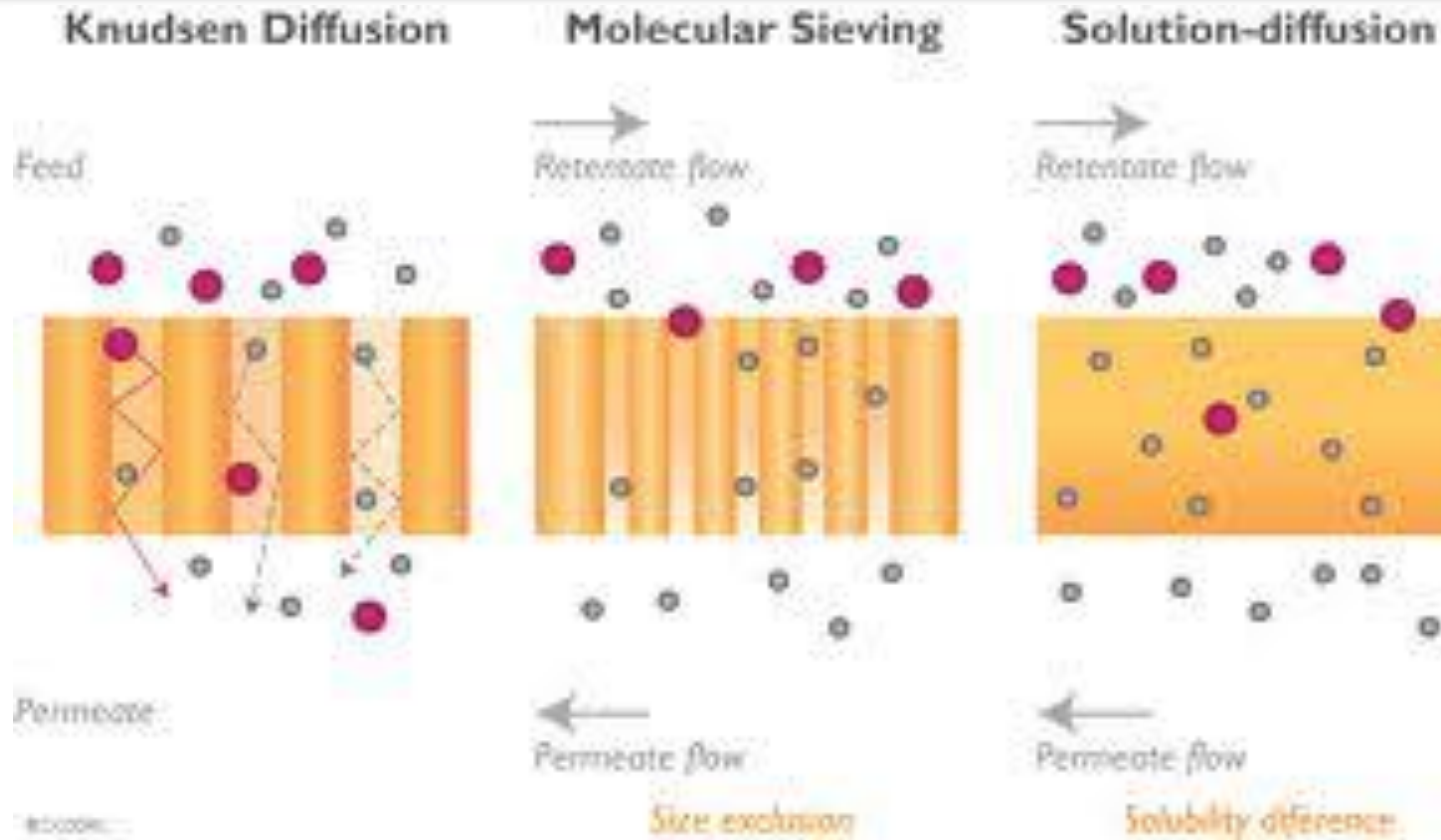


Key word is “safety”:

- evaluate the real-world environment that will impact the product,
- chemical exposure or contact solutions,
- temperature ranges,
- shielding,
- forces (including worst-case scenarios)
- **FUEL PERMEABILITY!**



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Permeability of vapour and liquids may lead by different mechanisms. The most common mechanisms are diffusion-solution model and Knudsen flow



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$$J = -D \frac{dC}{dl} = -D \frac{\Delta C}{\Delta l}$$

$$D = D_0 \exp\left(-\frac{E_d}{RT}\right)$$

$$C = S P$$

$$S = S_0 \exp\left(-\frac{H_s}{RT}\right)$$

$$J = D S \Delta P / l$$

$$Pe = Pe_0 \exp\left(-\frac{E_p}{RT}\right)$$

$$Pe = S D - \textit{permeability} \quad E_p = E_d + \Delta H_s$$

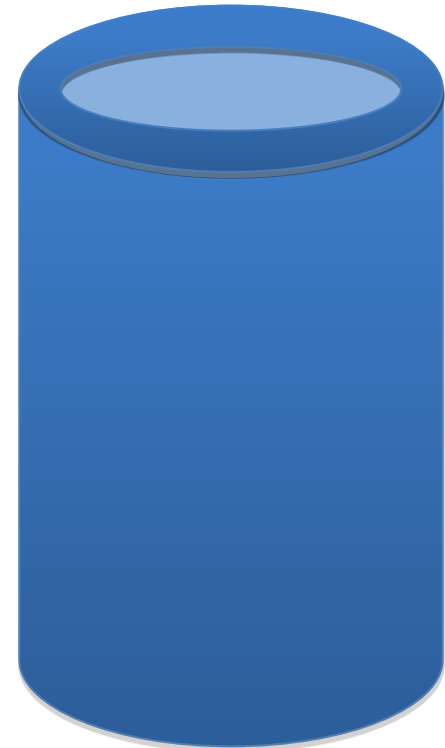


For the fuel evaporation thought the polymeric is calls pervaporation.

Pervaporation is membrane process in which the permeation of certain components through a polymeric film from a liquid feed mixture into a vapour phase is combined with the evaporation of these components.

The diffusion equation in cylindrical coordinates:

$$\frac{\partial C}{\partial t} = D \left(\frac{\partial^2 C}{\partial t^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{\partial^2 n}{\partial z^2} \right)$$



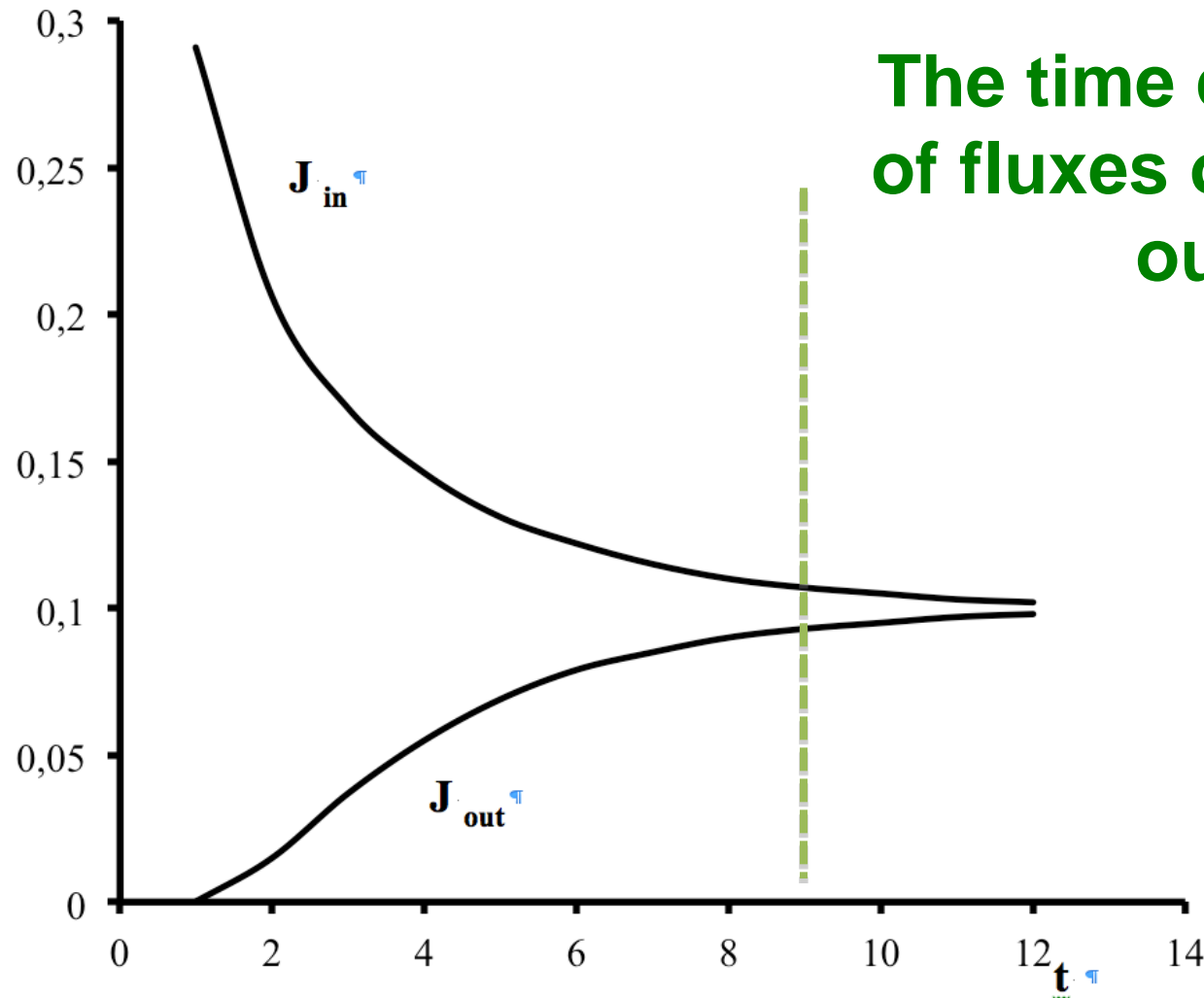


$$J_z = D \frac{\Delta C}{l} 2\pi r l \tau$$

$$J_r = D \frac{\Delta C}{\Delta \ln r} 2\pi l \tau$$

$$(\tau l^2/D) \ll 1$$

Monte Carlo Method
Molecular Dynamic



The time dependence
of fluxes on input and
output



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VERIFICATION



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$$J_z = D \frac{\Delta C}{l} 2\pi r l \tau$$

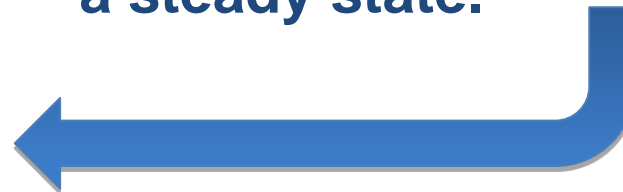
$$J_r = D \frac{\Delta C}{\Delta \ln r} 2\pi l \tau$$

$$(\tau l^2/D) \ll 1$$

$$J = \frac{3,83 \cdot 10^{-4}}{t + 7,66}$$

In the surface layer of the PTFE the concentration C is equal to the equilibrium concentration of the component in PTFE at the normal condition ($P=1$ bar).

In the longitudinal direction with a concentration of $l=0$ and $J_c=0$. Assumed that at the initial concentration corresponded equilibrium solubility, i.e. permeation process has reached a steady state.



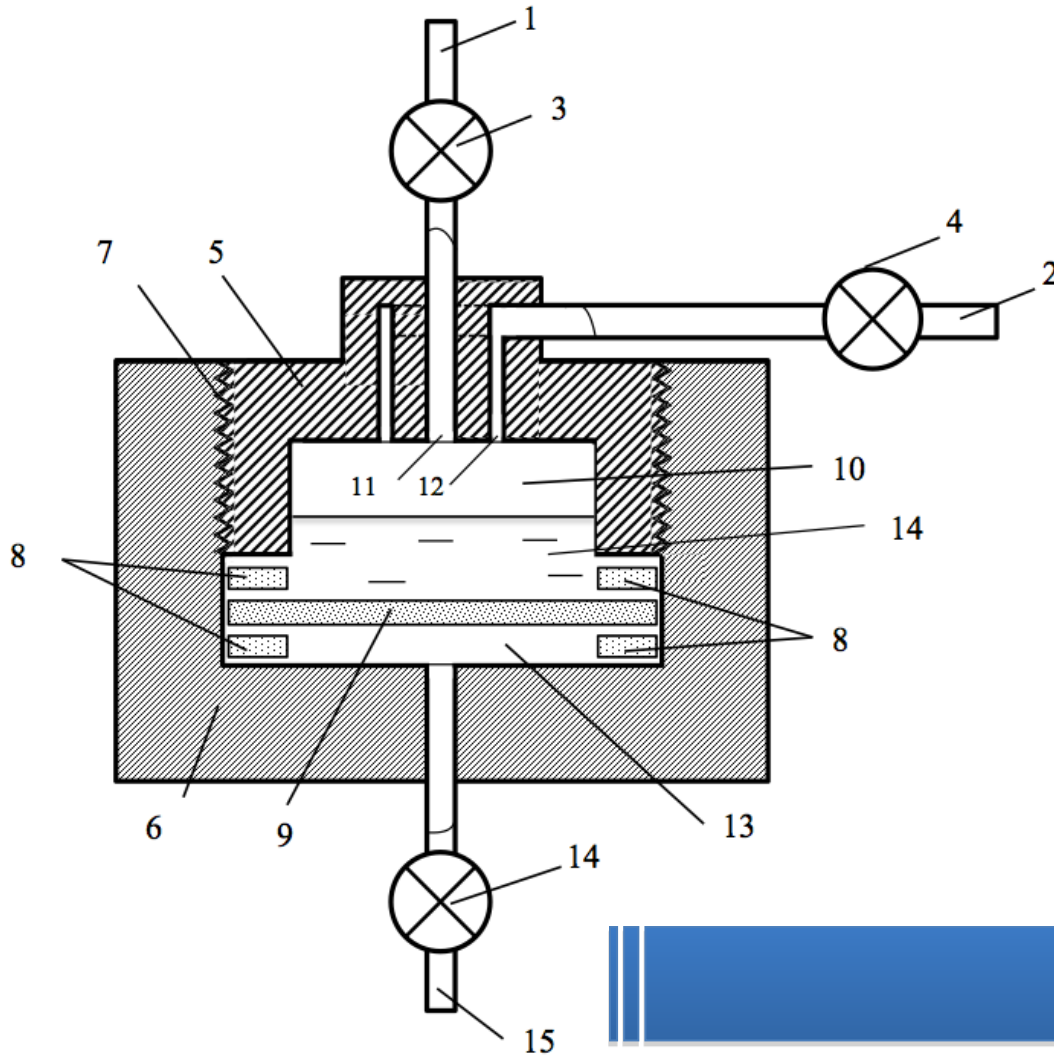
VERIFICATION



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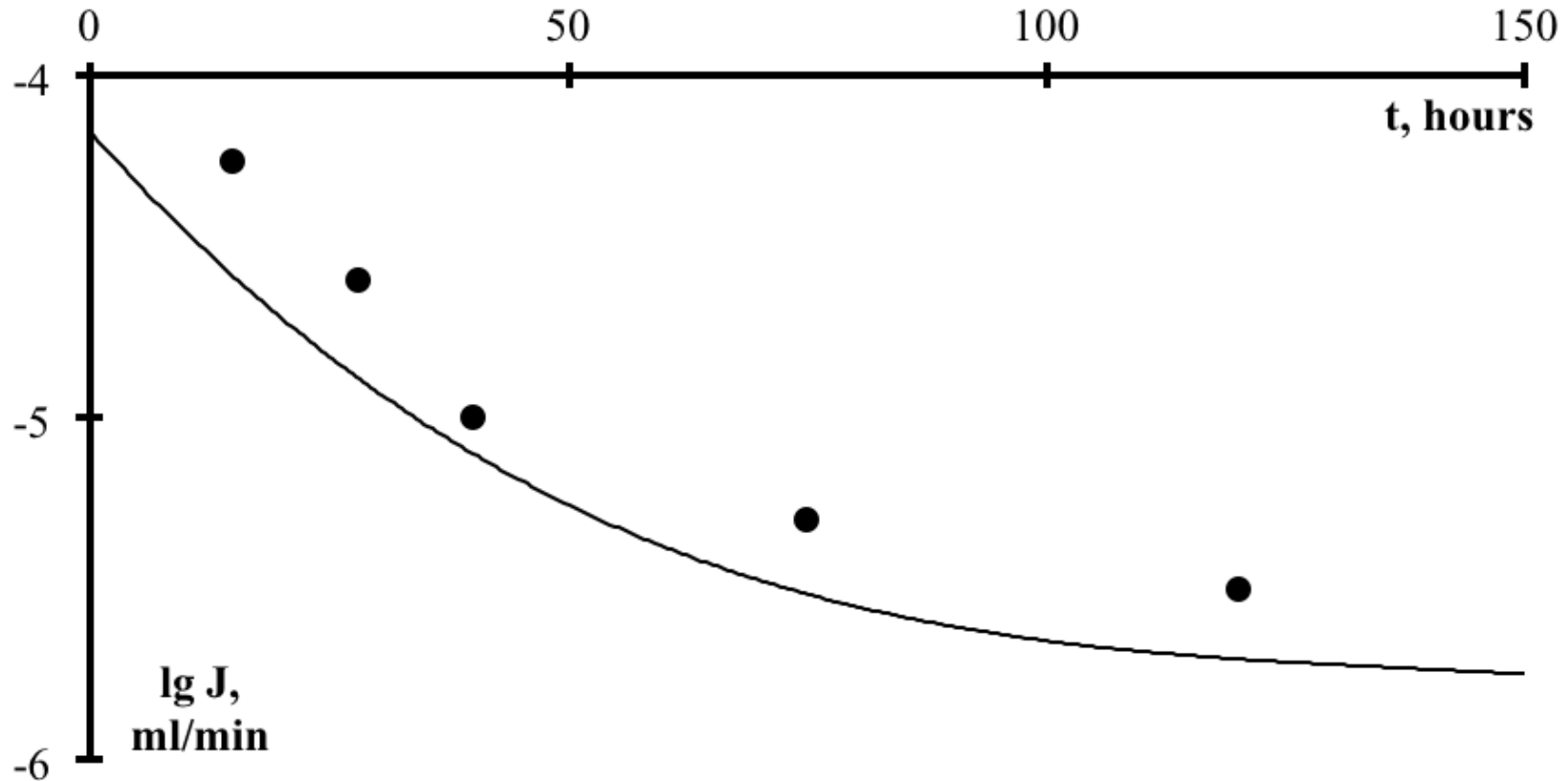
Testing module



VERIFICATION



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The experimental results (dots) and calculation by obtained equation

A slight deviation of the experimental data from the calculated due to the fact that in the calculations was considered homogeneous polymer and $D=8.8 \cdot 10^{-12} \text{ m s}^{-2}$.



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CONCLUSION



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The new approach for testing new polymeric materials was observed. The comparison theoretical and experimental data shows applicability of this procedure for automobile industry, especially developing of light commercial vehicle.



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Thank you for kind attention!
Welcome with your question...

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