The rarefied gas flow through a grid of cylinders

M. Yu. Plotnikov

*Institute of Thermophysics SB RAS,
Novosibirsk, Russia*

Motivation

Method HW CVD (hot wire chemical vapor deposition) is widely used for thin film deposition from the gas phase.
The method involves two stages:

1) activation of the gas on metallic wires;
2) deposition of the activated particles on the target.

When using the method for different gases it is necessary to solve the problems of two types:

1) to ensure maximum delivery of the activated particles to a target surface;
2) to provide the necessary proportion of particles colliding with the target.

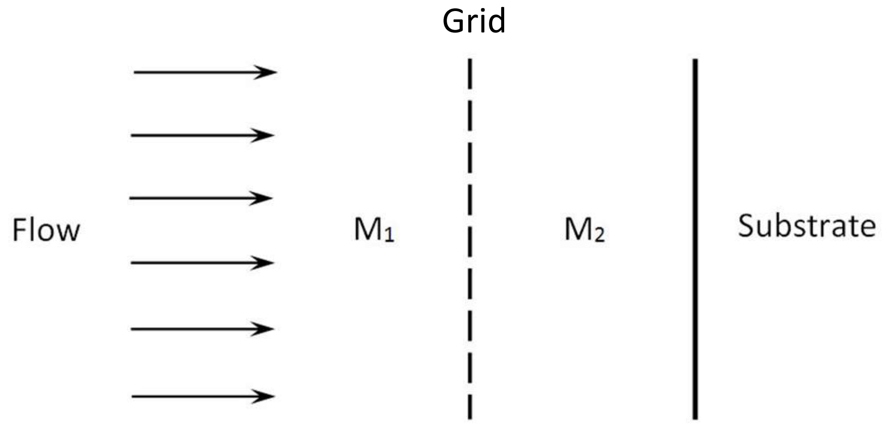
For this it is necessary to take into account
1) the impact of gas dynamics on the degree of gas activation on the wire surface;
2) change the number of activated particles due to possible chemical reactions in the gas phase.

Objective

This work is focused on finding ways to optimize a deposition of films from rarefied gas flow passing through the grid of heated cylinders, which is an activator.

The main efforts are focused on study the dependence of the relative number of dissociating particles on the degree of rarefaction, velocity of flow and the dissociation coefficient.

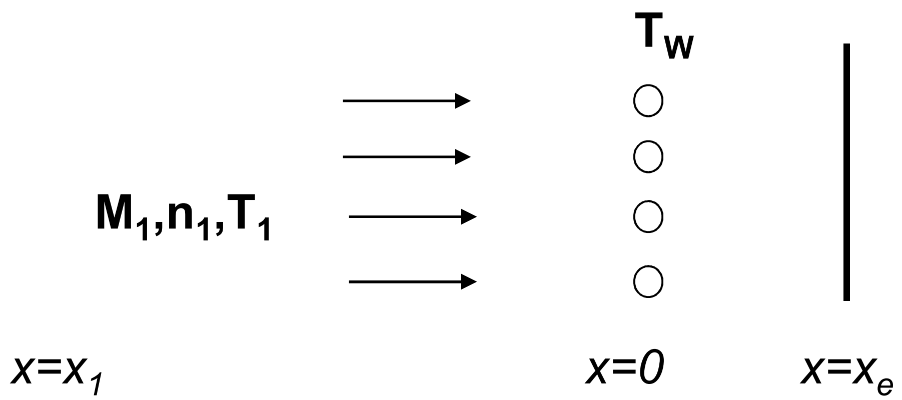
Configuration problem



It is clear *a priori* that the following flow regimes can be formed:

a) supersonic flow ahead of the grid and behind the grid $M_1>1$; $M_2>1$;
b) supersonic flow ahead of the grid and subsonic flow behind the grid $M_1>1$; $M_2<1$;
c) unsteady supersonic flow ahead of the grid and steady subsonic or supersonic flow behind the grid;
d) subsonic flow ahead of the grid and behind the grid $M_1 < 1$; $M_2 < 1$;
e) subsonic flow ahead of the grid and supersonic flow behind the grid $M_1 < 1$; $M_2 > 1$.

Formulation of the problem for supersonic flow



The initially undisturbed supersonic gas flow is directed toward the permeable obstacle. Parameters of flow are temperature T_1, Mach number M_1, and number density n_1.

The flow source is located in the plane $x=x_1$, the axes of symmetry of the cylinders composing the grid are located in the plane x=0, and the completely absorbing surface is located in the plane $x=x_e$. The diameter of the cylinders (**d**) and the distance between the axes of symmetry of the cylinders (**h**) are given.

An important characteristic of the problem is the possibility of particle pass through the grid without interacting with the surface of the wires (permeability **P=1-d/h**).

The value P close to 1 corresponds to a grid with a very big step between the wires.

The value P=0 corresponds to a continuous obstacle.

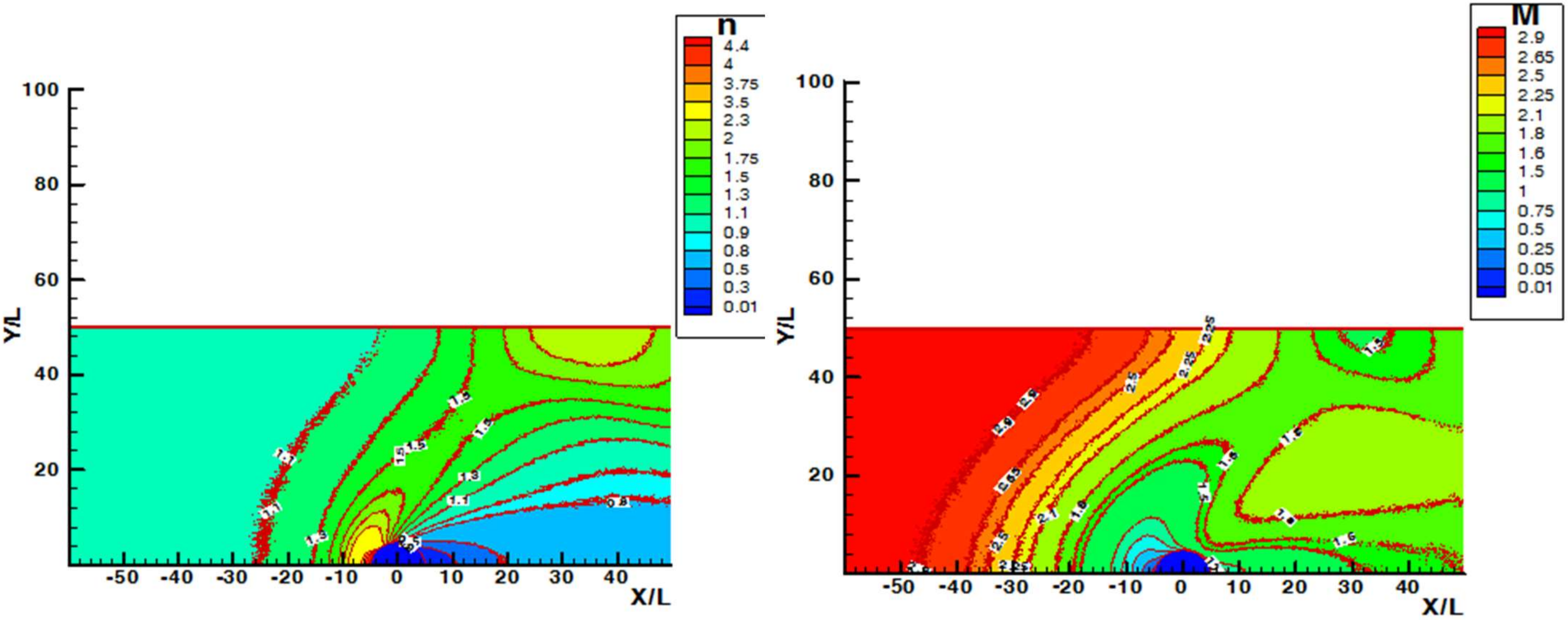
Solution by DSMC method

The problem is solved by the direct simulation Monte Carlo (DSMC) method [1]. The particle interaction is described by the model of variable soft spheres (VSS) with parameters corresponding to hydrogen [1]. When the hydrogen molecule interacts with the cylinder surface it split into atoms with a probability α. When the hydrogen atom interacts with the cylinder surface it recombs into molecule with a probability β. It was assumed that all particles are diffusely reflected from the surface with an energy corresponding to the temperature of the cylinder. Dissociation and recombination in the gaseous phase was not considered.

The governing parameters of the problem are the Mach number M_1, the Knudsen number Kn, recombination coefficient β, the dissociation coefficient α and permeability P.

[1] G. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Oxford, 1994

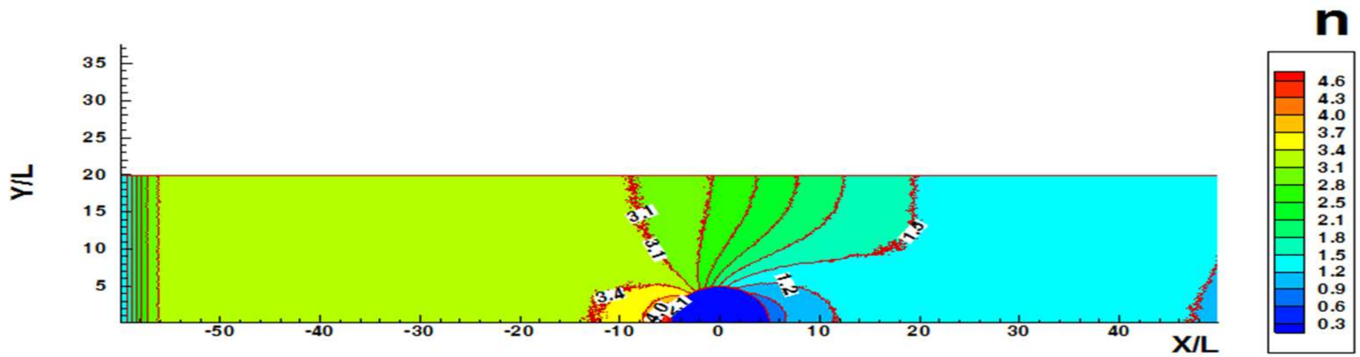
Spatial distribution of the flow parameters

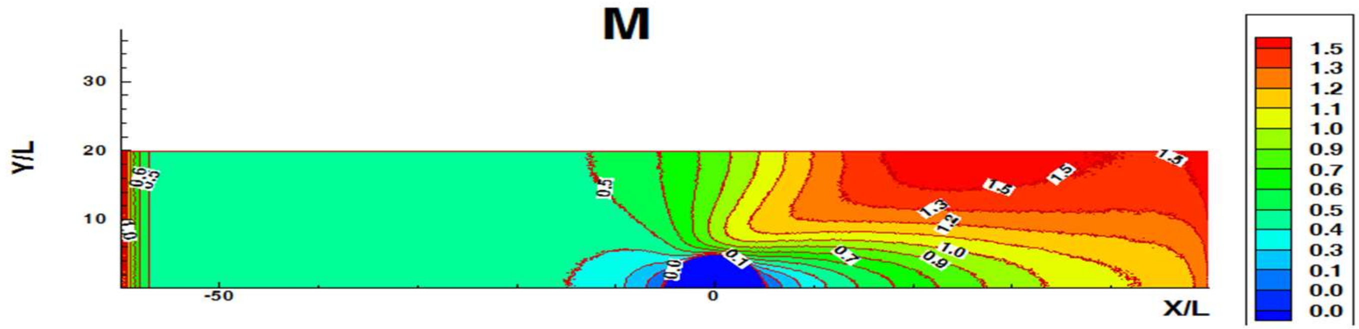


M1 = 3, Kn=0,1, P=0,9. Regime 1.

In a supersonic rarefied gas flow through an infinite periodic grid, located across the flow, there are two basic regimes. In the first case (regime 1), when the gas passes through the grid with a sufficiently large step between the wires, the separate shock disturbances are formed near each cylinder. A steady flow regime is organized there.

Spatial distribution of the flow parameters





M_1 = 3, Kn=0,1, P=0,75. Regime 2.

With a decrease of the distance between the wires, as well as at wire heating or increasing Knudsen number, there is a moment, when the supersonic flow cannot pass through the grid and some separate shock disturbances are combined into a plane shock wave, propagating upstream (regime 2). The problem becomes generally unsteady.

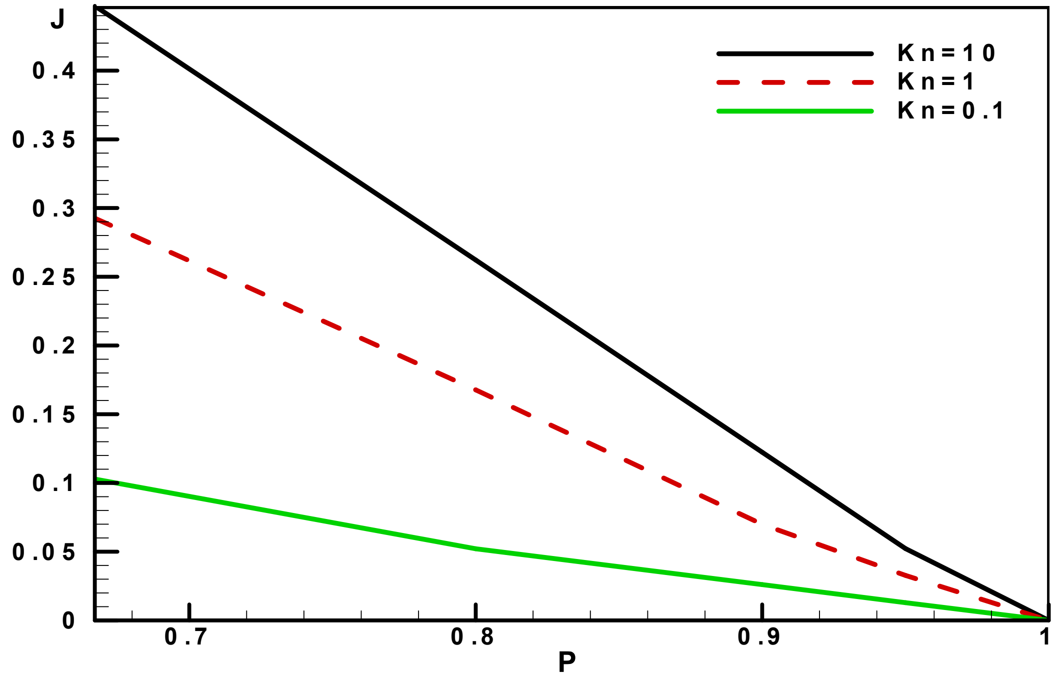
Numerical experiments

Numerical experiments were performed for the following set of parameters: $0.1<M_1<5$; $0,1 \le Kn<10$, $0<P\le1$, $T_w/T_1=2.2$. The conditions of numerical experiments have been focused on the experimental work with deposition of a diamond-like film [2,3]. Let J denotes the ratio of the number of atoms N_H passed through the cross-section $x=x_e$ to the total number of particles, passed through this cross-section: $J=0.5N_H/(0.5N_H+N_{H2})$

Cross section $x = x_e$ can be treated as deposition surface.
Numerical analysis showed that the obstacle permeability, Knudsen number, the flow velocity, and the degree of dissociation substantially affect on the value of J.

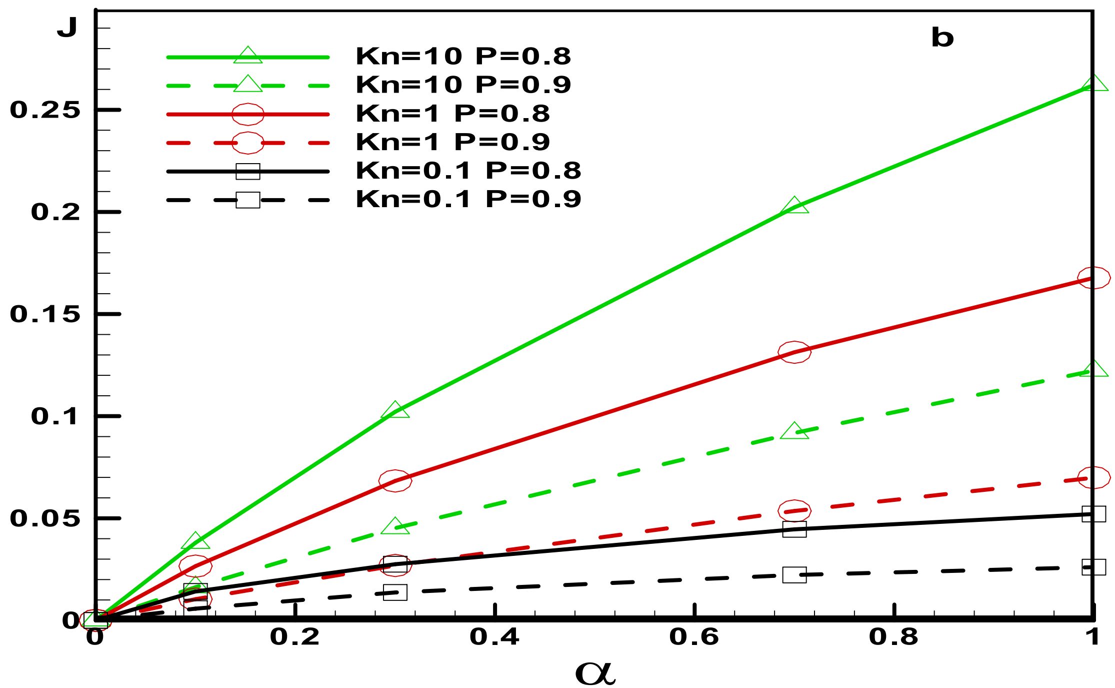
2. V.A. Volodin, A.A. Emel’yanov, A.K. Rebrov, N.I. Timoshenko, I.B. Yudin, *Journal of Engineering Physics and Thermophysics*, **85**, (2012).
3. A. K. Rebrov, A. A. Emel'yanov, I. B. Yudin, *Doklady Physics* **58**, № 5, (2013).

Dependence of ratio J on permeability P. M_1 = 3; α=1.



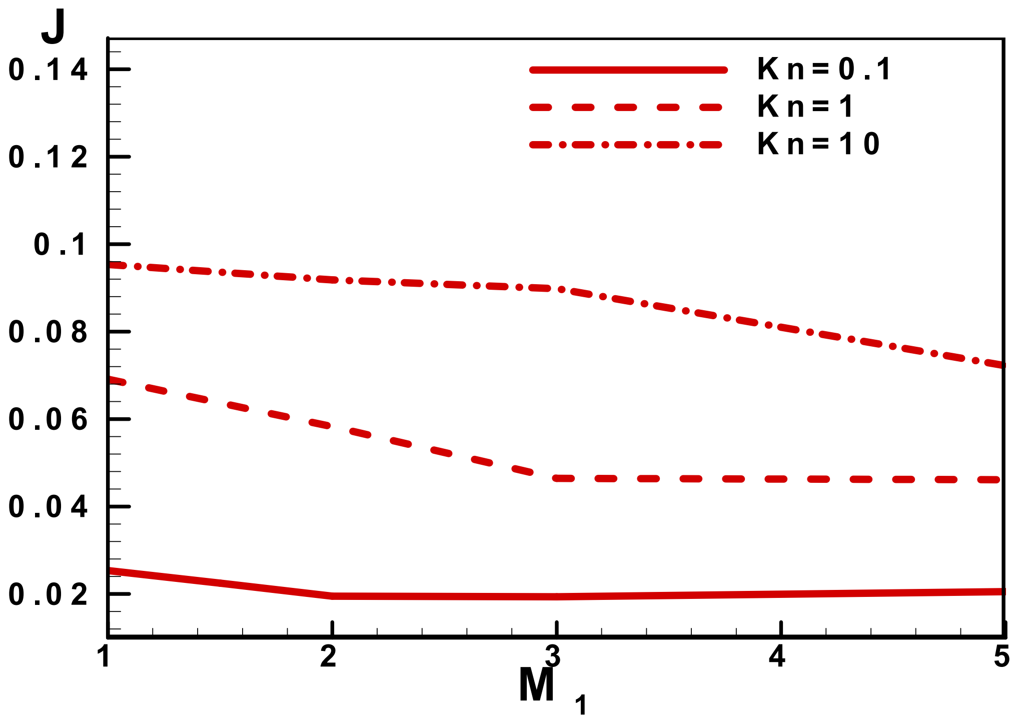
It can be seen that with a decrease in permeability value from P=1 to P = 0.85 ÷ 0.9 an increase in J occurs almost linearly. In this case the steady flow is generated. With a further decrease in permeability P=0.9 to P=0.85, the steady flow is reorganized into the unsteady one (regime 2). At further reduction in the permeability value, J increases, and at Kn=1 and 10 it increases almost linearly.

Dependence of the ratio J on α for different values of the Knudsen number.



We can note relatively linear change of the ratio J at $\alpha > 0.1$.

Dependence of the ratio J on the Mach number.



The flow velocity has a little influence on the number of dissociated particles in the case of supersonic flow.

Boundary conditions

1) A formal approach: the particles colliding with cross sections $x=x_1$ and $x=x_e$ are absorbed.

2) Conditions on the left boundary (cross sections $x=x_1$):

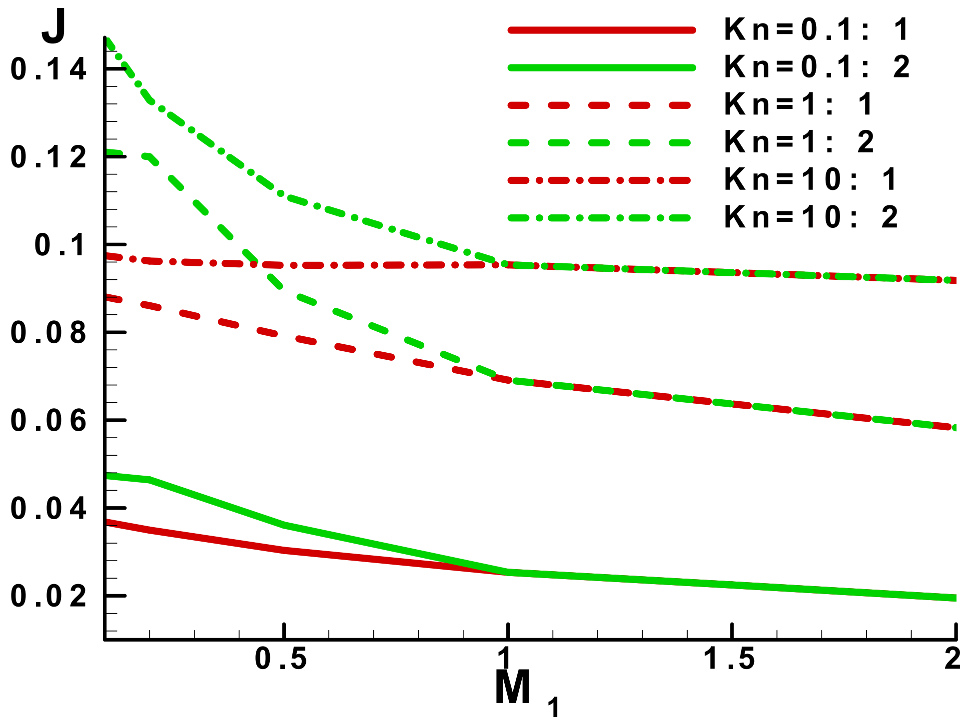
- If the particle H2 is returned to the source plane, it is absorbed;
- If the particles H are returned to the source plane, their reflection occurs with an energy corresponding to the velocity and temperature of the undisturbed flow.

Conditions on the right boundary (cross sections $x= x_e$):

- If the particles reach the plane $x = x_e$, their absorption-reflection is simulated according to the velocity and temperature of the undisturbed flow.

Setting of such boundary conditions provides given average flow velocity.

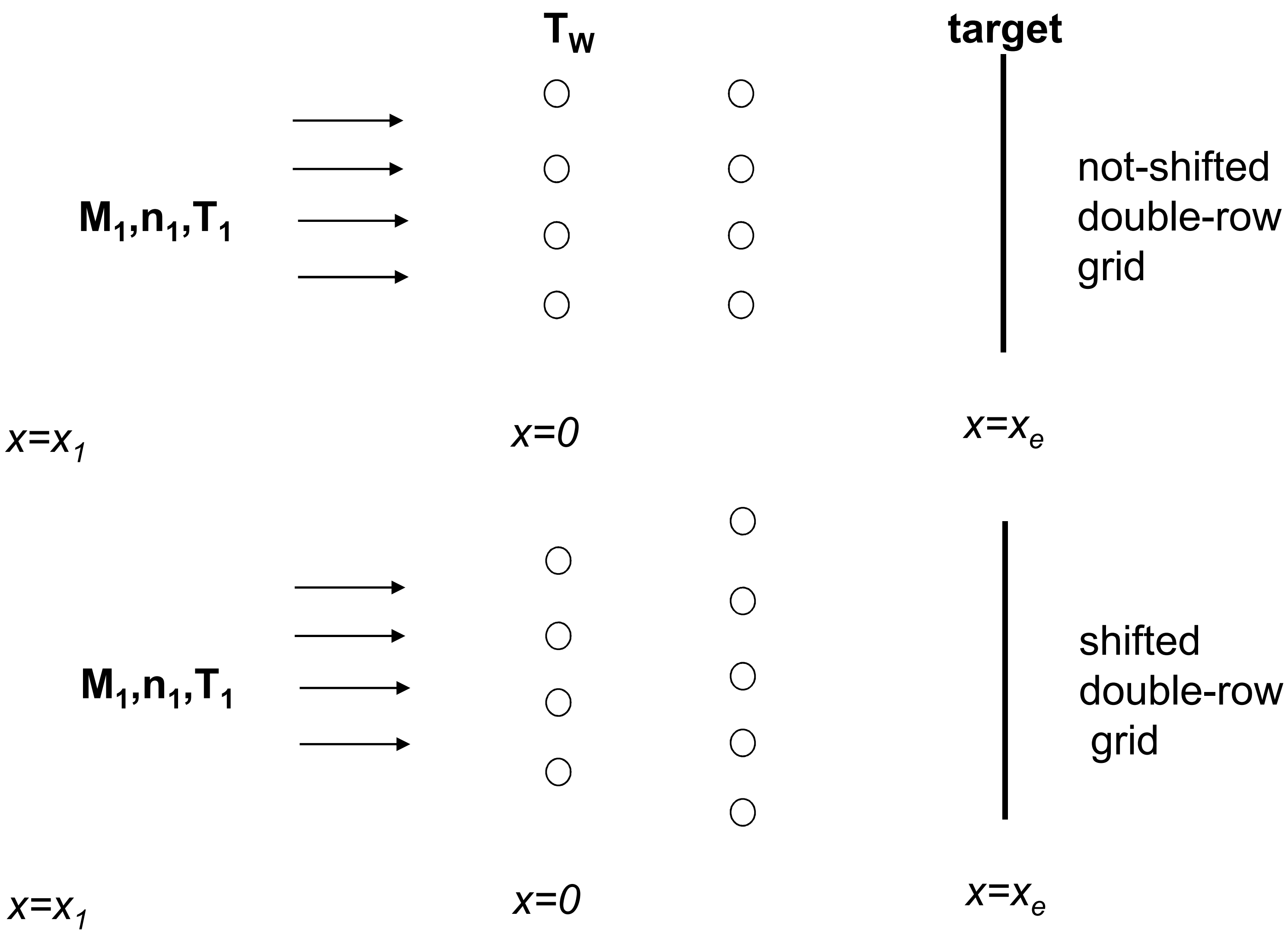
Dependence of the ratio J on M_1



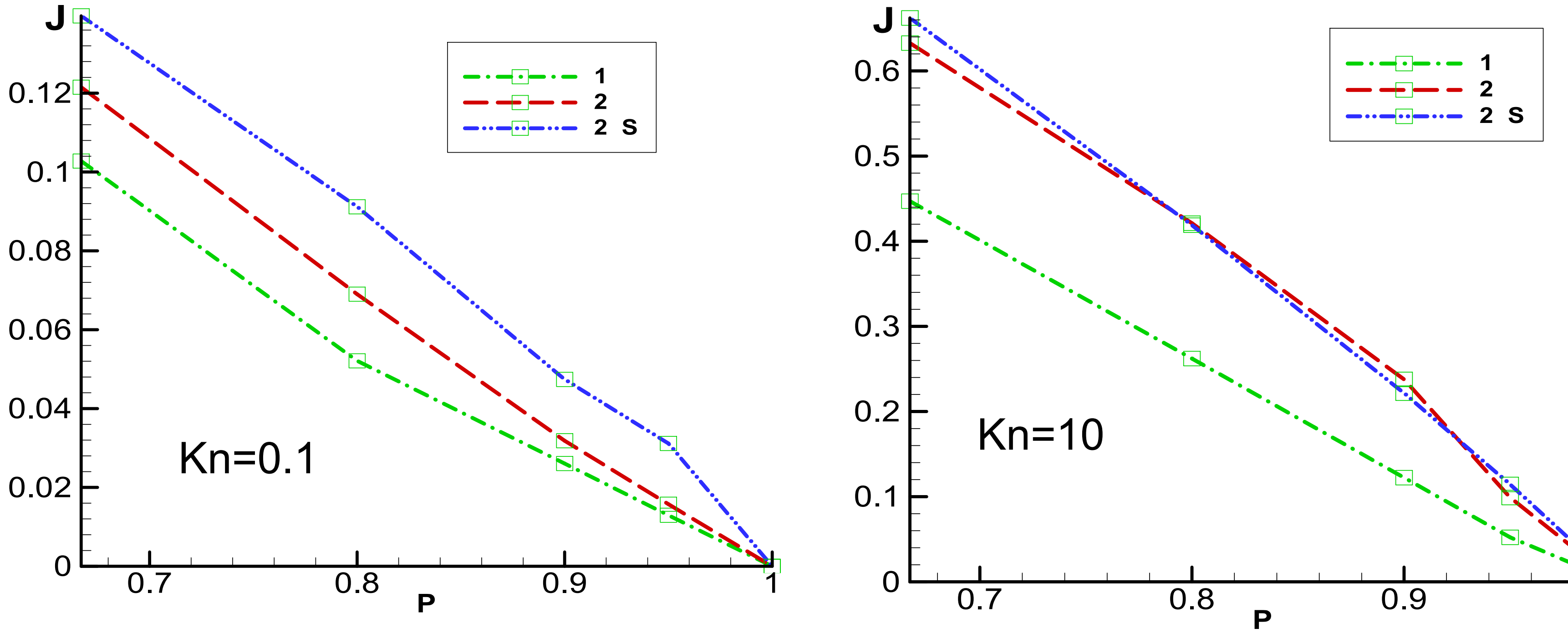
Curves 1 – first boundary conditions, 2 –second boundary conditions. α =1.

Decreasing of the Mach number leads to substantial growth J in the case of subsonic flow. This growth is more considerable in the case of the second boundary conditions.

Problem geometry: double-row grid.



Dependence of the ratio J on P. $M_1 = 3$.



Curves 1 – single-row grid, 2 –double-row not-shifted grid, 2S — double-row shifted grid.

The use of a double grid leads to an increase in the number of dissociated particles. For low Knudsen numbers the use of the shifted grid leads to optimal results. The use of the not-shifted grid gives the intermediate results because the second row of wires is in the rarefaction zone, formed at the flow around the wires of the first row. For the high Knudsen numbers a shift of the grids has no a significant effect on the number of dissociated particles.

Dissociation-recombination model

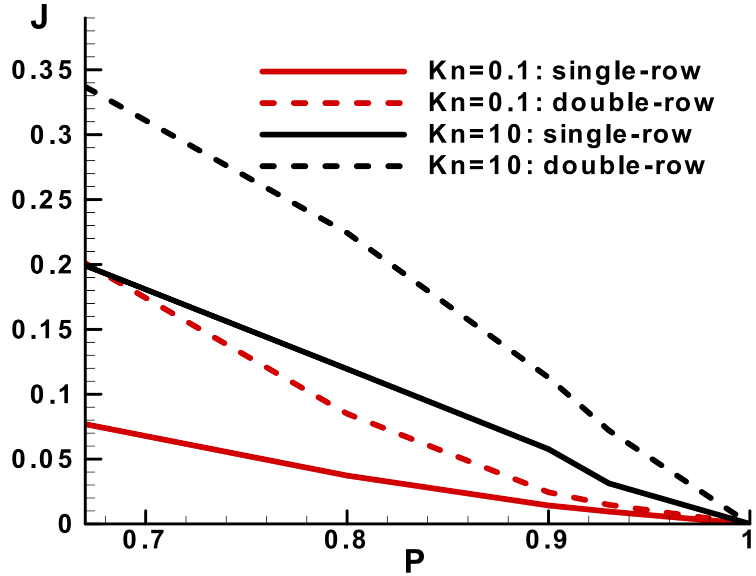
Analysis of experimental data and theoretical literature (26 articles) has led us to the following model of interaction of hydrogen with the tungsten surface at temperature of about 2400 K:

1) The hydrogen molecule dissociates into atoms with the probability α=0.4 and is specularly reflected with the probability (1- α) = 0.6 in collision with the surface.

2) The hydrogen atom recombines with the probability β=0.3, and is specularly reflected with the probability (1-β)=0.7 in the collision with the surface.

The particles arising from dissociation - recombination evaporate from the surface with a complete accommodation of momentum and energy.

Dependence of the ratio J on P for dissociation-recombination model .



Dependence of the ratio J on P for single-row and double-row not-shifted grid. M_1 = 3.

We should note a relatively linear J change at P > 0.92 (regime 1) and P < 0.92 (regime 2).

Conclusions

For the considered range of flow parameters, the character of a change in the number of dissociated particles was determined depending on rarefaction degree, flow velocity, permeability obstacle and degree of dissociation. It was established that:

- the portion of dissociated particles increases with the Knudsen number;

- in the case of flow separation (formation of the subsonic zone near the obstacle - regime 2), the portion of dissociated particles increases significantly;

- the use of a double-wire grid allows an increase in the number of dissociated particles.

- the flow velocity has a little influence on the number of dissociated particles in the case of supersonic flow; decreasing of the flow velocity leads to substantial growth in the case of subsonic flow.

The greatest influence on the number of dissociated particles has permeability obstacle.

Thank you
for your attention!