Development of a Simulation Code for ITER Vacuum Flows

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Abstract. The ITERVAC code, newly developed at Forschungszentrum Karlsruhe, has become an essential tool for validation of proposed design changes to the ITER vacuum pumping systems (neutral beams, torus exhaust, cryostat high vacuum systems and dedicated forepump trains), which are characterised by transitional flow conditions. Because of the importance attributed to the calculation results of ITERVAC, the code must be extensively benchmarked. The benchmarking exercise was successfully done in the field of laminar and free molecular flow; however, it has been found that literature data for the transitional flow range, which is of prime relevance for the ITER conditions, are scarce and even not existing for geometries as complex as for the ITER vacuum pumping ducts. Therefore, a comprehensive programme was started to provide a parametric benchmark data base. This work includes significant efforts to develop new solutions in the field of kinetic theory, and is complemented by the set-up of the dedicated experimental facility TRANSFLOW. This paper starts with an outline of the basic ideas behind the ITERVAC code. In the second part, new results based on kinetic theory are presented and the experimental facility is described.

1. Introduction and Background

ITER features three large vacuum pumping systems for evacuation and maintenance of the required pressure levels in the cryostat, the torus, and the neutral beam injectors (NBI), respectively. Especially the latter two systems are characterized by very high gas flows, which are to be pumped.
As described in the ITER outline design [1], the NBI cryopump vacuum system has to provide an average pressure of 0.2 Pa in the injector, and 0.02 Pa in the neutralizer region, against a gas flow of 41 (Pa·m³)/s, which is currently considered to be further increased by 25%. The reference design of the ITER torus exhaust pumping system is based on 8 cryopumps, connected via 4 ducts to the torus, each of them containing a pump in direct line of sight and a branched pump [2]. Due to the small burn-up fraction, the total gas throughputs are very high, control of which, especially for the helium ash, is one of the key issues affecting the performance and achievable burn time of a fusion reactor. The design governing requirement for the torus exhaust vacuum pumping system is to maintain a pressure level between 1 and 10 Pa in the divertor private region at a maximum gas flow of 153 (Pa·m³)/s.
The flow through a vacuum system is characterized by the interactions between the gas molecules themselves and between the molecules and the surrounding walls. Based on that, different regimes can be defined, using the dimensionless Knudsen (Kn), Reynolds (Re) and Mach (Ma) numbers, see Table I. The gas flow through the ITER vacuum systems covers a wide range of Kn numbers, starting from continuum and slip in the gas sources (divertor, NBI injector), covering transitional flow for the ducts, and ending up in free molecular flow regime inside the cryopumps. A reliable assessment of the throughput of such a vacuum system therefore requires a tool to describe the whole range of rarefied gas flows. As indicated in Table I, the viscous regime can be calculated relatively well, either with well approved engineering formulae, based on solutions of the simplified Navier-Stokes equation, or with CFD codes, and the molecular flow is usually treated with high accuracy using Monte Carlo codes.

TABLE I: GAS FLOW REGIMES.

Range of Kn	Flow regime	Governing equations	Numerical approach
Kn → 0	Continuum (invscid)	Euler	Typical CFD schemes
Kn < 10^{-3}	Continuum (viscous)	Navier-Stokes	
10^{-3} < Kn < 10^{-1}	Slip	Navier-Stokes with slip flow boundary conditions	
10^{-1} < Kn < 10	Transition	Boltzmann and kinetic models	Analytical methods (1D), Variational methods, Discrete velocity methods, Integro-moment method, DSMC
10 < Kn	Free molecular	Boltzmann and kinetic models without collisions	Method of characteristics, Test particle Monte Carlo

The problem comes from the transitional flow range, for which the existing methods include high computational efforts. In order to validate quickly any modifications introduced to the vacuum system in the detailed design, it would therefore be essential to have an easy-to-use code, which is valid for arbitrary channel cross-sections and lengths over the whole range of Kn number and is able to illustrate promptly how the system performs with any design change. The driver for the work presented in this paper was to develop such a general tool to describe ITER vacuum flows (ITERVAC).

2. Basic Framework of the ITERVAC code

Since the pioneering work of Knudsen, it is known that the gas flow rate through a prismatic duct shows a typical minimum in certain ranges of the Knudsen number. The local Knudsen number is defined as the ratio of the mean free path (at the given temperature and local pressure of the gas species flowing through the duct) and hydraulic diameter d_h. The latter is defined as 4 times the cross-section over the wetted perimeter; for a circular duct, it becomes identical to the diameter.
Figure 1 (left) shows the well-known gas flow characteristics through a long circular channel in non-dimensional form. The function F is a dimensionless mass flow $\dot{m}$, defined as

$$F = -\dot{m} \cdot \frac{8 \cdot \sqrt{2 \cdot k \cdot T / m_0}}{\pi \cdot d_h^3 \cdot (\partial p / \partial x)} \quad . \tag{1}$$

Here, m_0 is the molecular mass of the gas and k is the Boltzmann constant; the pressure gradient $(\partial p / \partial x)$ refers to the axial direction x.
This dimensionless relation is widely used in rarefied gas dynamics and is (for given boundary conditions) primarily a function of just one parameter, the Kn number. The basic, and in the first instance purely empirical idea behind the new code was to start from the curve shown in Fig. 1, and to describe that with a general fitting function. A functional analysis delivered several possibilities to do that, out of which the following one with four parameters c_i was finally considered to be most promising:

$$F = \frac{c_1}{Kn} + c_2 + \frac{c_3 \cdot Kn}{c_4 + Kn} \quad . \tag{2}$$

With eq. (2) the points shown in Fig. 1 could be fitted with a maximum error of less than 3%. The general idea now is to apply eq. (2) for all prismatic channels using the hydraulic diameter for generalization. As basic requirement, it must first be shown that the chosen function F fulfils the physical boundaries for continuum and free molecular flow.

2.1. The free molecular flow limit

For sufficiently high Knudsen numbers, the limit of free molecular flow, F_{mol}, has to be met:

$$\lim_{Kn\to\infty} F = c_2 + c_3 = F_{mol} \quad . \tag{3}$$

In the case of a free molecular flux of particles following Maxwellian distribution, there holds the following general expression for the mass flow of a gas with the particle mass m_0 through an arbitrary duct between the inlet cross-section A_1 and the outlet cross section A_2:

$$\dot{m} = m_0 \cdot (I_1 \cdot w_{12} \cdot A_1 - I_2 \cdot w_{21} \cdot A_2) \quad , \tag{4}$$

with the incidence

$$I = p / \sqrt{2 \cdot \pi \cdot k \cdot m_0 \cdot T} \quad , \tag{5}$$

and the molecular transmission probability w_{ij} in direction i→j. Assuming $A_1=A_2$ and $w_{12}=w_{21}$ (prismatic, isotropic, isothermal channel), and subsequent insertion of (4) and (5) in the definition equation (1) yields the following expression for the limit flow F_{mol} :

$$F_{mol} = \frac{w_{12} \cdot A \cdot 8 \cdot L}{\pi^{3/2} \cdot d_h^3} \quad , \tag{6}$$

which simplifies to

$$F_{mol}^{circ} = \frac{2 \cdot w_{12} \cdot L}{d \cdot \sqrt{\pi}} \quad , \tag{7}$$

for the circular duct of a length L. Coupling of eqs. (3) and (6), or (7) respectively, delivers an expression to calculate $(c_2 + c_3)$.

On the basis of Fig. 1, which indicates an asymptotic constant F_{mol} for high Knudsen numbers, it becomes obvious that the product term w·L/d must become a constant for sufficiently long channels. We have performed Monte Carlo simulations for high L/d ratios and estimate the limit value for L/d→ infinity to be around 2.57 for the circular duct.

2.2. The viscous flow limit

For sufficiently low Knudsen numbers, the laminar flow limit has to be met asymptotically:

$$\lim_{Kn\to 0} F = c_1 / Kn = F_{visc} \quad . \tag{8}$$

For the long circular duct, there results the viscous limit (Hagen-Poiseuille solution) with:

$$F_{visc} = \frac{4 \cdot \sqrt{\pi}}{Kn \cdot \mathrm{Re} \cdot \xi} \quad , \tag{9}$$

with the friction factor ξ. Coupling of the latter two eqs. defines c_1. In the case of laminar flow (ξ=64/Re), there results $c_1 = (\sqrt{\pi}/16)$.

By introducing the generalized c_{lam} concept [3], there results the following expression for c_1, holding for arbitrary prismatic channels:

$$c_1 = \frac{c_{lam} \cdot 16 \cdot A}{\sqrt{\pi} \cdot d_h^2 \cdot \mathrm{Re} \cdot \xi} \quad . \tag{10}$$

2.3. Interpretation of the factors c_i

As shown above, c_1 describes the viscous limit, and (c_2+c_3) is strongly correlated with the free molecular limit. In the following section, we try to separate c_2 and c_3, and interpret c_4 .

Based on the addition theorem for reciprocal conductances [4] under free molecular conditions, it can be illustrated that c_3 indicates the beaming effect of the molecular flow through the channel [5]. The beaming effect describes the sorting of the moving directions of the flowing particles such that there results a directed flow at the outlet of the duct, even if there is Maxwellian distribution at its inlet. This is simply due to the fact that small reflection angles from the wall produce considerably longer flight paths along the axial coordinate of the duct. This effect is more pronounced the longer the duct is. The contribution of transport by this effect to the overall molecular flow limit is given by $c_3/(c_2+c_3)$; this is 22.8% for the fully developed molecular flow through a long circular pipe. The parameter c_4 indicates the Kn number at which the beaming effect contribution is just 50% of the Kn→∞ limit c_3. A parameter variation study showed that fixing c_4=1.4 yields the best results. Table II lists the parameters for several example geometries. Figure 1 shows the corresponding curves as a function of Kn.

ITERVAC does also describe short ducts (L/d<80). In these cases, c_2 and c_3 are weighted by a free molecular correction function, and c_1 has to include entrance effects (cf [5]).

2.4 ITERVAC networking

The ITERVAC code does not only provide a description of the flow through a single duct, but also allows to model a complex vacuum system (which we have in case of ITER) by a network of connected ducts. The ITERVAC code allowed, for the first time, a systematic analysis of the ITER vacuum pumping systems; it has been recently applied to estimate gas density distribution inside the NBIs [6]. By modelling studies performed for the ITER torus exhaust vacuum pumping system several weaknesses in the duct design could be revealed [7]. An example for a modeling network is shown in section 4 below.

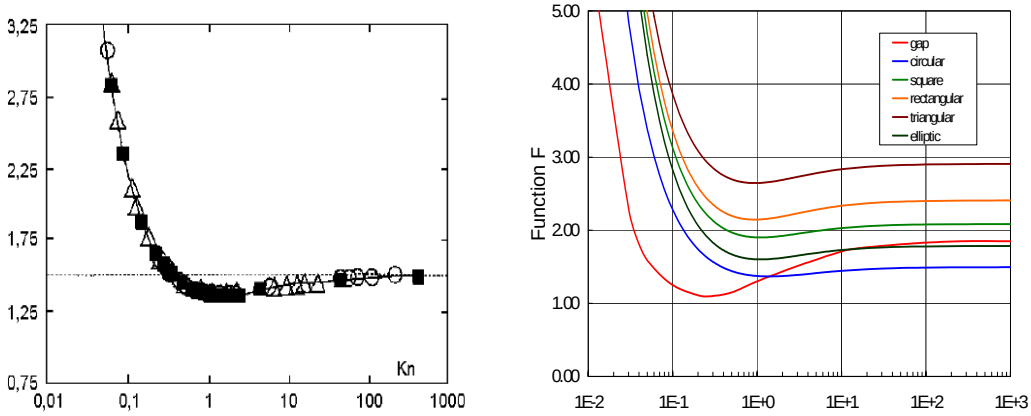

FIG. 1. Non-dimensional mass flows at high L/d ratios as a function of the Kn number: Experimental values for the flow through cylindrical ducts (left) [8], ITERVAC calculated flows for various cross-sections (related to the length for the gap with infinite cross-section) (right).

TABLE II: PARAMETERS c_i FOR THE ITERVAC CODE.

Geometry	c_{lam}	c_2	c_3	c_4
Circular	1.0	1.1162	0.3291	1.4
Square	1.12462	1.4862	0.5735	1.4
Rectangular (2x1)	1.02907	1.6655	0.7318	1.4
Triangular	1.2	1.9706	0.9632	1.4
Elliptic (2x1)	0.95108	1.3404	0.5054	1.4
Infinite gap	2/3	0.7133	1.1918	1.4

3. Benchmark of the code

Due to the potentially very significant implications of the ITERVAC results on the ITER design, it is absolutely essential to benchmark the code. An efficient benchmark has to include different geometries and different flow ranges. It must also include short and long ducts. The code benchmark must include experimental literature values as well as other theoretical approaches (compare Table I).
For a circular pipe and a number of other geometries, closed analytical solutions (Navier-Stokes equation solutions) as well as many experimental data are available in the viscous flow regime. But also here, the situation becomes very complex, as soon as it comes to short channels. The molecular flow regime in all geometries and L/d ratios can be very well and reliably treated by Monte Carlo methods, in case of a circular pipe even closed analytical solutions are available. However, for the ITER relevant transitional flow range, even for the simplest geometry of a long cylindrical pipe, experimental data are extremely scarce and do not seem to be very reproducible. Fortunately, kinetic solutions do exist for some geometries (circular at large and small L/d; rectangular).

3.1. Solutions based on kinetic theory

As it is pointed out in the introduction, kinetic type approaches are very efficient in solving vacuum flows in the whole range of the Kn number. In this approach the Boltzmann equation or reliable kinetic model equations are solved numerically. Even more, when the flow is fully developed or otherwise the ratio of the length over the hydraulic diameter of the channel is much larger than one, the governing kinetic equations are linearized and then very accurate results may be produced with modest computational effort. In the University of Thessaly, Volos, significant progress has been made in this field. In this context, recently, the flow of single gases and binary mixtures, through tubes [9,10] and ducts [11,12] has been solved. This is why a collaboration has been started between Volos and the vacuum system designers at Forschungszentrum Karlsruhe.
The numerical solution is obtained by using the discrete velocity method (DVM). The kinetic equations are discretized in the molecular velocity and spatial spaces and then, they are solved in an iterative manner. For small values of the Kn number the convergence rate of the iterative map is very slow and in these cases an accelerated version of the DVM is applied [13]. At the boundaries the gas–surface interaction is modeled by the Maxwell interaction law assuming purely diffuse reflection and by taking the accommodation coefficient $\alpha = 1$. It is well known that this type of reflection is valid only for rough surfaces and heavy gases, while in the cases of smooth surfaces and light gases $\alpha < 1$. It has been found experimentally that usually $0.6 \le \alpha \le 1$.
Here, we present recent results of single gases and binary mixtures through cylindrical tubes and orthogonal ducts by considering diffuse and specular reflection at the wall. The flow is due to an imposed pressure gradient and the kinetic models, proposed by Sakhov and McCormack for single gases and binary mixtures respectively, have been applied. In Figure 2, we present the non-dimensional flow rates for these problems with $\alpha = 1$ (purely diffuse) and $\alpha = 0.8$ (80% diffuse and 20% specular) in terms of the rarefaction parameter δ, which is proportional to the inverse Kn number $\delta = \sqrt{\pi}/(2 \cdot Kn)$. The results for the single gas are valid for any monoatomic gas. For the binary mixture case, we have chosen to present the results of He-Xe, with a molar concentration of 0.5, because for this particular mixture we have noted a large departure from the corresponding single gas results. This is due to the large ratio of the molecular masses of the two species.

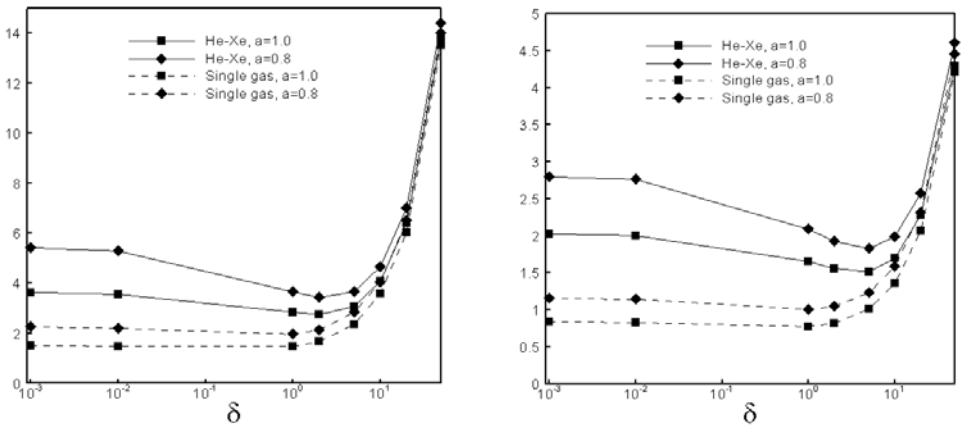

FIG. 2. Non-dimensional flow rates for single gas and equimolar binary mixture (He-Xe) through a cylindrical tube (left) and rectangular duct (right)

It is seen that the non-dimensional flow rates depend significantly on the value of the accommodation coefficient. As the coefficient α is decreased the flow rate is increased. In addition, the departure on the estimated flow rates between $\alpha = 1$ and $\alpha = 0.8$, for small values of δ (free molecular regime) is about 30-40%, and then as δ is increased and we are getting into the transition regime this departure is reduced and finally is completely eliminated as we are approaching the continuum limit (large δ). It should be noted however, that the qualitative behavior of the flow rates in terms of δ for $\alpha = 1$ and $\alpha = 0.8$, including the Kn minimum, remains the same. Based on these results, a more concise and complete comparison with experimental results, taking into account the roughness of the surface, is under way.

3.2 Benchmark results

Until now, three fields have been assessed for benchmarking:

1. Viscous flow through long and short circular and triangular equilateral channel: The average error found was in the order of 3%.
2. Molecular flow through several channel shapes (circular, square, triangular, rectangular) at varied length to diameter ratio L/d. The maximum error found here was 3%.
3. Transitional flow through a circular tube at varied L/d ratio (from orifice to very long). The ITERVAC results were compared with kinetic theory solutions [14]. For a long pipe the deviation of calculation against simulation found was about 20 % in some cases, only 5% in other cases. For a thin orifice a deviation of about 8 % was found at 10 Pa upstream pressure, increasing up to 40%, especially in the low diameter region, at an upstream pressure of 1 Pa (Fig. 3).

In summary, the benchmark so far revealed a very good agreement of the ITERVAC code in viscous and molecular flow range. In transitional flow range, there are larger discrepancies, however without obvious trends. The ITER divertor duct system is characterized by channels with complex shape (conical, trapezoidal) and at short L/d (around unity). To develop solutions for short ducts based on kinetic theory are one of the major challenges in that field. This is why it has been agreed to start a next step, which is the experimental verification of ITERVAC simulations with a new dedicated test rig TRANSFLOW (Transition Flow Range Experiments). The philosophy is to provide a broad parametric and relevant range of well defined experimental data which can be used to benchmark the code.

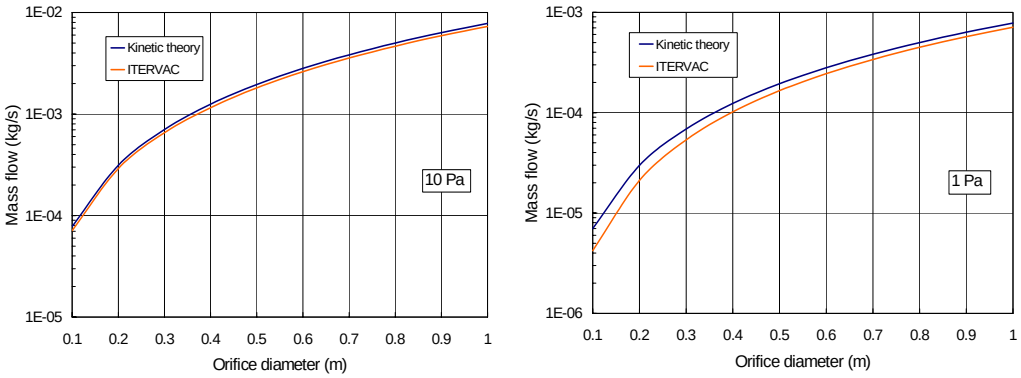

Fig. 3. ITERVAC results vs. calculated mass flows through an orifice at an upstream pressure of 1 Pa and 10 Pa, respectively (Tritium, 273 K).

4. Experimental work in TRANSFLOW

The experimental aim of the activities in TRANSFLOW is to measure the mass flow through interchangeable test channels in a broad range of Re, Kn and Ma numbers, and to compare the results against predictions from ITERVAC analysis and kinetic theory calculations. The extension of these kinetic calculations to channels of various cross sections is under way.
The test rig can be separated into the dosing dome, two adapter flanges with the test channel in between and the pump dome (Fig. 4). The dosing dome serves the purpose to produce an isothermal flow at a constant pressure difference through the test channel. The pump dome holds all pumps (two 2800 l/s turbomolecular pumps, one 250 m³/h screw forepump, one 800 m³/h roots pump).
During measurement the adjusted gas flow is dosed into the dosing dome via a mass flow controller or a calibrated orifice, depending on the needed range. Different transducers register pressure and temperature inside the dome. The gas flow path comprises the first adapter flange, the test channel, the second adapter flange, the pump dome, and finally the turbomolecular pumps with the forepumps. The real flow path has been modelled by means of 24 ITERVAC unit cells of different geometry (Fig. 4, right). The measurements will take place at isothermal conditions. The facility is commissioned for non-flammable gases. The typical pressure inside the TRANSFLOW test rig is in between 100 Pa and 10^{-6} Pa, depending on the channel length. The temperature range is in between ambient and 200°C.

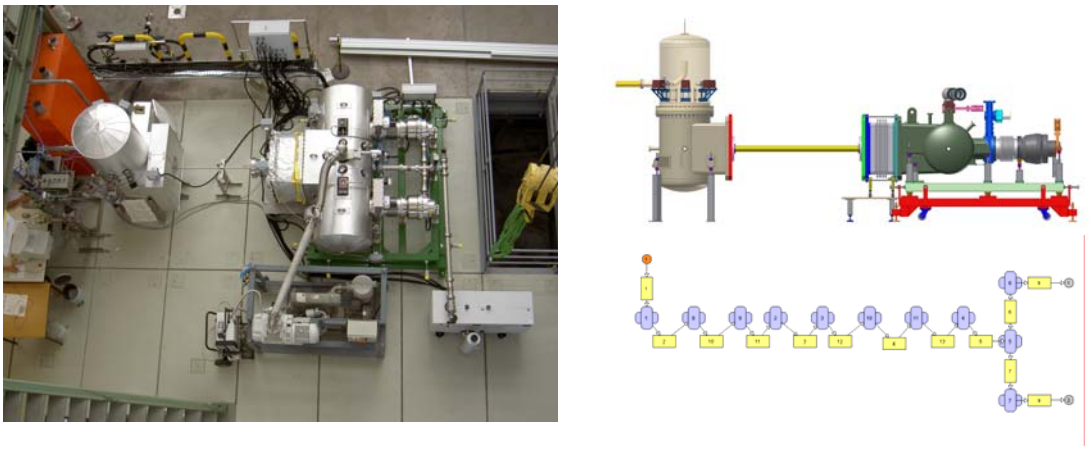

Fig. 4 The TRANSFLOW facility. Bird´s eye view (left); Illustration of the ITERVAC model network of the facility, to derive the flows through the test channel (right).

For temperature regulation a heating system of both domes, the adapter flanges and the test channel is installed. The experiments can be done in fully automated way, involving PLC control and data acquisition. The operation of the facility has started with a long circular pipe (L/d=80, d_h=16 mm); the behaviour of this channel is well-known so that these measurements can be used to validate the experimental approach itself. It will be continued with more complex channels (short and long, elliptic, trapezoidal, square, triangular).

5. Conclusion and Outlook

Significant progress has been made in the development of the ITERVAC code to describe the ITER vacuum systems, which are typically operated in transitional flow conditions. Due to the essential importance of the code results to the baseline ITER design, a comprehensive programme for code benchmark and validation has been initiated. This comprises ITER relevant experimental work for defined channels and theoretical work in the field of the kinetic theory. ITERVAC will not only be used to optimise the torus exhaust and NBI vacuum systems, but will also become an important design tool for the divertor flows (on the neutral side), where it will be used to identify and optimise bypass leaks.

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