

# A Molecular Theory of the Onset of Turbulence

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## ABSTRACT

We review experimental data which shows the dependence of the critical Reynolds number on molecular composition. We then use the cell model of a gas to explain the onset of turbulence by the excitation of the internal degrees of freedom of molecules. Two sources of internal energy states are identified: quantum confinement for monoatomic molecules and rotational states for diatoms.

*Keywords:* turbulence, Reynolds number, molecules

The Navier-Stokes equation from the continuum model of hydrodynamics is a very successful equation for describing laminar flow. It is also used extensively, but not so successfully, for describing turbulent flow (Frisch, 1995). For this reason, it may be useful to adopt a molecular approach as an alternative. Recent experiments (Novopashin & Nerushev, 1997; Someria, 1999) seem to support the idea that turbulence may have a molecular origin, instead of a flow, or mathematical provenance, as conventionally accepted. If a molecular origin for the onset of turbulence is established, this will put into question the exclusive use of the continuum model expressed by the Navier-Stokes equation for understanding turbulence. A molecular approach in simulating hydrodynamics has also been developing (Koplik & Banavar, 1995; Flekkoy & Coveney, 1999), illustrating for example, how molecular dynamics may be brought to the level of dissipative particle dynamics. This is of some interest to our own works (Muriel & Dresden, 1995; Muriel, 1998), which require radiation as a mechanism for dissipation to arrive at some turbulent-like behavior. For these reasons, we summarize relevant experimental

results to date, and further interpret and describe our molecular theory of turbulence presented earlier in several mathematical papers (Muriel & Dresden, 1995; Muriel & Dresden 1996; Muriel & Dresden 1997; Muriel, 1998), to arrive at a simple interpretation of the theory. With this paper, we will also suggest further experiments to test our ideas.

The molecular view of the onset of turbulence could be surprisingly simple. When mechanical or thermal agitation of a fluid is sufficiently strong, the internal degrees of freedom of the molecules are excited. Part of the kinetic energy of motion of molecules arising from fluid flow is converted to energies of collision, by some process of partial equipartition. If this energy is sufficient, a diatomic molecule, for example, could become excited, and give up radiation in the process – a turbulent fluid is known to heat up.

There is of course the question of noble gases which are simple enough to be modeled as point masses participating in fluid flow. They too become turbulent. We shall address this problem shortly. We will start with molecules with easily identifiable internal degrees of freedom.

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Consider a diatomic molecule with rotational states. An excited diatomic molecule gives up radiation, ultimately a quantum phenomenon with built in stochasticity. The direction of the radiation can only be described probabilistically. By conservation of momentum and energy, the molecules recoil stochastically as well. The stochasticity we are discussing here is different from the stochasticity contributed by an external heat bath. We identify this small stochastic contribution to molecular recoil velocities to provide the onset of turbulence. This stochastic velocity is propagated and magnified in a turbulent fluid. In this way, we find a physical origin for the Reynolds decomposition of fluid velocity into a regular and stochastic component (Reynolds, 1883). Heretofore, the Reynolds decomposition has been justified by the existence of turbulence, one must acknowledge its stochastic contribution by inserting the decomposition. It is also a mathematical approach that does not prescribe from first principles when such a decomposition begins. In contrast, we propose here that the Reynolds decomposition is dictated by the physics of excitation. Historically and mathematically, it is only after the Reynolds decomposition is assumed that one can begin to model turbulence (McComb, 1991). For this reason, we suggest that the Navier-Stokes equation alone cannot describe the entire range of laminar, laminar-turbulent, and turbulent regimes, without putting turbulent-like solutions first.

To introduce our reasoning, we summarize the energies of various molecules which participate in fluid flow and their excitations:

(1) Diatomic molecules in their ground states have rotational energies of the order of  $8 \times 10^{-16}$  erg ( $5.03 \times 10^{-4}$  eV). Note also that room temperature  $kT$  is roughly  $4.09 \times 10^{-14}$  erg ( $2.57 \times 10^{-2}$  eV). We can see that rotational energy excitations and de-excitation are well within the range of a room temperature gas.

(2) An argon atom participating in fluid flow with an average velocity 20 cm/sec has an energy of  $1.33 \times 10^{-20}$  erg ( $8.4 \times 10^{-9}$  eV). By increasing the velocity to at least tenfold (around 350 cm/s), one may increase the energy to  $10^{-18}$  erg ( $10^{-6}$  eV) — we should take note of this energy for consideration later in this paper.

But to return the case of noble gases, where there are no rotational states, what would be the corresponding excitation states? We answer this question shortly.

In the meantime, let us first look at the Novopashin data in Fig. 1 and Table 1.

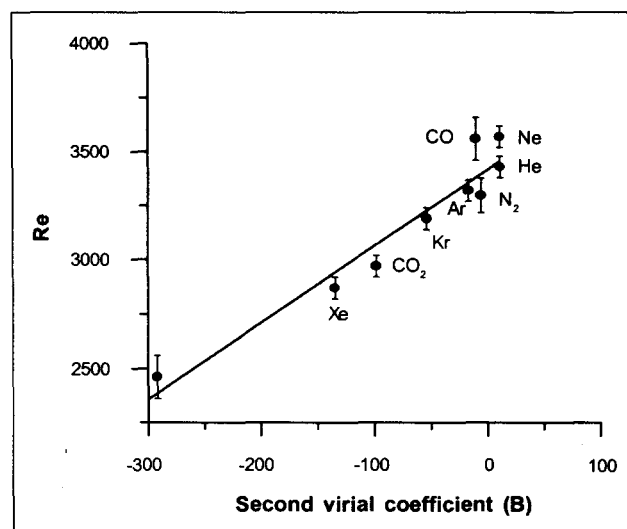


Fig. 1. Critical Reynolds number versus second virial coefficient plot for some monoatomic and diatomic gases.

Molecule	Rec	Dynamic Viscosity (m <sup>2</sup> m/s)	Atomic mass (amu)	Density	(At. Mass/Density) <sup>4/3</sup>	Rec*Dynamic Viscosity <sup>4/3</sup> (At. Mass/Density) <sup>4/3</sup>
He	3430	19.9	4.003	0.1785	63.24	4316572
Ne	3570	31.75	20.18	0.900	63.23	7166962
Ar	3320	22.75	39.95	1.784	63.12	4767453
Kr	3190	25.54	83.80	3.73	63.40	5165363
Xe	2870	23.3	131.3	5.897	62.64	4188799
CO2	2970	15.0	44.01	1.977	62.62	2789721
CO	3560	17.9	28.0	1.25	63.14	4023533
N2	3290	17.9	28.014	1.25	63.19	3721322
SF6	2530	15.9	146.06	6.5	63.40	2550391

Table 1. Critical Reynolds numbers for mono-atomic and diatomic gases.

First, the dependence of the critical Reynolds number on the second virial is clear. Since the second virial is the first dominant term of the departure from ideal gas behavior, Fig. 1 is proof of the molecular dependence of the onset of turbulence.

Second, consider the data in Table 1. The 5th column shows that the product of the critical Reynolds number, dynamic viscosity, and the molecular mass to the 4/3 power divided by the density to the 4/3 power is of the same order of magnitude for like gases. Why is this so?

To answer the last question, we look back at a very early and successful application of quantum mechanics to the ideal gas, the cellular model (Hill, 1960), which reproduces all the results of the thermodynamics of ideal gases. This model assumes that a molecule or atom is caged by a box of other molecules, which is taken as a simple cube of dimension, where  $\nu$  is now the kinematic viscosity

$$L = \left( \frac{m}{\rho} \right)^{1/3}$$

where  $m$  is the molecular mass and  $\rho$  is the density. from quantum mechanics, the energy of this molecule is given by

$$E = \frac{h^2(n^2 + m^2 + l^2)}{8mL^2}$$

where the quantum numbers  $n, m, l$  run from 1 to infinity and  $h$  is Planck's constant. Using the quantum states above, the thermodynamics of an ideal gas can be completely derived (Hill, 1960).

We now use the cell model as a mental construct to explain turbulence. Consider a molecule caged by its surrounding molecules. The cage and the molecule inside may be moving bodily with a fluid velocity  $\nu$ . When the fluid velocity is increased, part of the molecular velocities is converted to kinetic energies of collision. However, according to our picture, part of this kinetic energy of motion is converted to mutual

collisions which result in the excitation of the caged molecule. Although such collisions are obviously complex, we continue to adopt the cell model, but introduce the excitation of the caged molecule. This allows the caged molecule to be excited to an internal energy state given by  $E$ . Now the lowest energy transition of the caged molecule from one state to another is given by

$$\Delta E = \frac{3h^2}{8m} \left( \frac{\rho}{m} \right)^{2/3}$$

which will have to be overcome by the energy due to collisions. According to our model, a critical fluid velocity is needed to overcome this energy, given by

$$\alpha m \nu_c^2 = \Delta E$$

where  $\alpha$  expresses the unknown fraction of the energy drawn from the fluid kinetic energy that is converted to the excitation energy of the molecule. This equation connects the macroscopic fluid velocity to the internal energy states of the molecules. The internal energy is given by quantum confinement as in the cell model. Substituting the gap energy, we get the following critical velocity

$$\nu_c = \frac{h}{m} \left( \frac{\rho}{m} \right)^{1/3} \sqrt{\frac{3}{8\alpha}}$$

from which we obtain the critical Reynolds number

$$\text{Re}_c = \frac{\rho \nu_c d}{\eta} = \frac{hd}{\eta} \left( \frac{\rho}{m} \right)^{4/3} \sqrt{\frac{3}{8\alpha}}$$

where  $d$  is a typical dimension of the turbulence apparatus and  $\eta$  is the dynamic viscosity.

If we now perform identical laminar-turbulent transition experiments on two different pure gases using the same apparatus, we can form the ratio

$$\frac{\text{Re}_{c1}}{\text{Re}_{c2}} = \left( \frac{\rho_1}{\rho_2} \right)^{4/3} \left( \frac{m_2}{m_1} \right)^{4/3} \left( \frac{\eta_2}{\eta_1} \right) \left( \frac{\alpha_1}{\alpha_2} \right)$$

Now if the molecular geometry is the same, the two  $\alpha$  cancel, and we get the following relation for similar molecules

$$\text{Re}_c \eta(m/\rho)^{4/3} = \text{Re}_c \nu m^{4/3} / \rho^{1/3} = \text{constant}$$

Remarkably, we find that the above relationship is somewhat verified in Table 1. We know that the cell model agrees quite well with classical results in thermodynamics. Now, it seems to work as well as a check on empirical results in turbulence. The above analysis shows something else—that a quantum cell model also explains the onset of turbulence. Even more important, we do not always need to invoke an internal degree of freedom as in molecular rotation and its quantum states to find an energy gap argument. Quantum confinement arguments seems to be enough.

We illustrate this further. As we mentioned earlier, the molecular kinetic energy due to laminar flow is quite low. The energy of an argon molecule moving with a fluid at a velocity of 20 cm/sec is  $1.33 \times 10^{-20}$  erg ( $8.4 \times 10^{-9}$  eV). For argon, at a density of  $1.784 \times 10^{-3}$  g/cm<sup>3</sup>, we find that the quantum energy due to confinement is of the order of  $2.176 \times 10^{-18}$  erg ( $1.37 \times 10^{-6}$  eV). So by simply increasing the average macroscopic velocity of argon, as discussed earlier, we can attain the quantum of energy due to confinement. All of this could happen well below the room temperature  $kT$  of the order of  $10^{-14}$  erg ( $10^{-2}$  eV). So when the argon macroscopic fluid velocity begins to excite this quantum confinement energy, the gas becomes turbulent. In this way, we can explain all the data for noble gases, and surprisingly some of the data for other molecules despite the expected inequality of the unknown coefficient  $\alpha$  for molecules of different structure.

However, according to the above reasoning, since carbon monoxide and nitrogen have the same molecular

mass, density, as well as dynamic viscosity, the critical Reynold numbers should be the same, yet they have been found to be different (Nerushev & Novopashin, 1997). But for these two molecules, their rotational energy spectra are different, so when this rotational energies are also excited, there will be a rotational contribution to excitation, radiation, and turbulence. It is the molecule with a lower excitation state which gets turbulent sooner, in this case, nitrogen. Hence, a quantum confinement argument is supplemented by rotational excitation to display a difference in the onset of turbulence.

In fact, it appears that the rationale is the following. In any gas or liquid, we must look for the lowest form of energy excitations. This may well be quantum confinement or molecular rotation. Once the lowest energy spectrum is determined, we use it to define the onset of turbulence. But whatever it is, the onset of turbulence seems to have a molecular and, therefore, quantum origin.

All of the above arguments have originated from rather involved theoretical considerations (Muriel & Dresden, 1995; Muriel & Dresden, 1996; Muriel & Dresden, 1997; Muriel et al., 1998; Muriel, 1998), which provided the impetus to perform the experiments (Nerushev, 1997; Novopashin, 1998; Sommeria, 1999). Once this phase of theorizing and experimentation has begun, as in fact it has, it is possible to explore new features of this view of the onset of turbulence, independently of our early theoretical and experimental work. The classic quasi-static approach of Novopashin (1997 & 1998) and the dynamic free efflux experiment of Sommeria (1999) using ultrasound techniques may now be augmented by other experiments, like the measurement of the radiation spectrum of a turbulent gas, and the influence of radiation on the onset of turbulence, two other effects that we have predicted earlier (Muriel & Dresden, 1995). When this is done, it is possible to introduce to turbulence research some new techniques from ultrasound and molecular spectroscopy which can only enrich the field, and cultivate the hope of finally explaining turbulence from first principles of physics, instead of from mathematics alone.

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