

SOLID PROPELLANT MICROTHRUSTER: THEORY OF OPERATION AND MODELLING STRATEGY

*Evgenii B. Rudnyi, Tamara Bechtold and Jan G. Korvink
IMTEK, Freiburg University, Freiburg D-79110, Germany
C. Rossi*

LAAS-CNRS, 7 ave du colonel Roche, 31077 Toulouse cedex 4, France

Abstract

A modelling strategy for a microthruster array based on solid fuel is presented. We review the theory of operation of the microthruster that includes an electro-thermal process, ignition, sustained combustion, membrane rupture and gas dynamics. The recommended level of theory is chosen to answer practical engineering questions, so as to make the recommended models feasible to develop and optimize. Special attention is paid to transferring the resulting models to existing software for electrical circuit simulation to permit the development of intelligent electrical driving circuits. The methods of automatic model reduction are presented and the most appropriate method for a microthruster array is chosen.

Introduction

A new class of microthrusters is based on the integration of solid fuel with a silicon micromachined system (see Fig 1).¹ The principal feasibility of the approach has already been demonstrated by a number of research groups.^{2,3,4} The next step is to fabricate a working array of independently addressed solid propellant microthrusters on a single chip and then to optimize its performance.

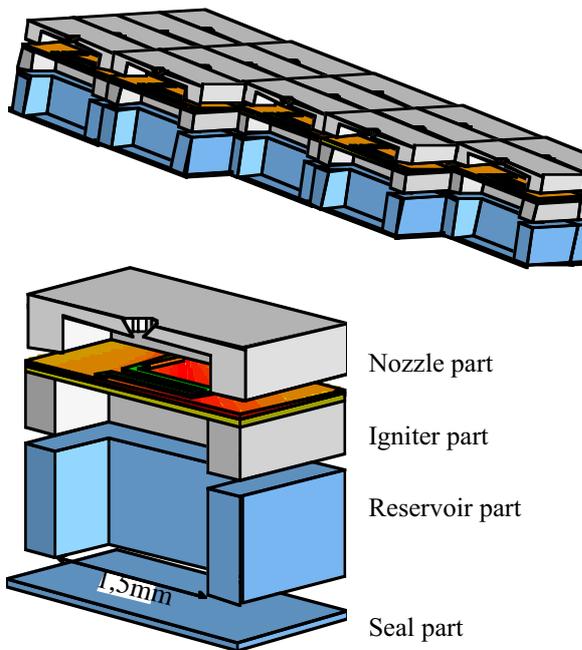


Fig. 1. Microthruster array and an individual device, technical details are presented elsewhere.²

The space community has much accumulated experience in modelling and simulating solid fuel rockets. We mention here an ambitious project to make a full-scale simulation for the whole solid propellant rocket.⁵ However, knowledge from macro-devices do not scale well for micro-devices. Effects that are usually neglected for the macroscale start to dominate on the microscale. As a result, macroscale material properties may not be valid for a microdevice and even the governing equations sometimes have to be modified. For example, the Knudsen number for the microchannels becomes relatively large and hence the conventional Navier-Stokes equations may not be valid.⁶ Another difference is a level of integration: a single chip will contain hundreds of microthrusters and it is necessary to exclude so-called “thermal crosstalk” between neighboring microthrusters. A microthruster device must be fired, but this event must not provoke the firing of other devices.

One of the reasons of moving for smaller sized satellites is cost reduction. This also means a smaller budget for the satellite development team. This requires a lot of interdisciplinary knowledge from a particular engineer taking part in the development of the microthruster. This is quite different from the development of a big rocket where different engineers are responsible for the manufacturing of different pieces. To this end, computer simulation appears to be very important. The software embeds the knowledge of previous generations of scientists and engineers and, if used with wisdom, it can significantly aid designers.

The present paper discusses all aspects of computer modelling related to the development of a solid propellant microthruster array. The main challenge is to identify the appropriate relationship between modelling and experiment. We will start the paper by a discussion of this problem. Then the governing equations, which are necessary to model the work of a single microthruster device, are reviewed. For each process, a hierarchy of available approximations is presented. Next, we recommend the most appropriate level of theory in order to answer practical engineering questions, so as to make the recommended models feasible to develop and to compute.

Special attention is paid to transferring the resulting models to existing software for complete transient microsystem modelling, or in other words, to system level simulations. This is very important for the devel-

opers of the electrical circuitry as they need to obtain the microthruster real-time response in order to develop an intelligent circuit. The main problem here is the high-dimensionality of the system of ordinary differential equations obtained after the discretization of the original governing equations. The methods of automatic model reduction are therefore reviewed and the most appropriate method for a microthruster array is chosen.

Modelling Strategy

The goal of any theoretical description is to obtain a mathematical model which can predict device behaviour within the desired accuracy. In order to solve the mathematical model one usually has to perform numerical computations, in other words, a simulation. Today, because of great scientific progress and Moore’s law for constantly increasing computing power there are number of possibilities, shown in Table 1, to start creating the model. Nevertheless, the deeper the level, the more computationally intensive the methodology.

There are ambitious modelling projects that start from first principles when the goal is to simulate complex systems without adjustable parameters,⁷ that is, based on the very basic laws of nature (Quantum chemistry and atomistic models in Table 1). Typically, here the goal is to solve the electronic Schrödinger equation in order to estimate potential energy surface for a given molecular system and then by means of molecular dynamics or Metropolis Monte Carlo to obtain all necessary material properties.⁸ The latter can be used in continuum-based models in Table 1 such as Navier-Stokes equations for macroscopic devices.

On the other hand, and not without ground, models based on a lumped representation still enjoy widespread use in the engineering community. Rocket engineers are sceptical about possibilities to solve Navier-Stokes equations for reactive multiphase flow,⁹ not even speaking about molecular dynamics. They prefer to use much simpler models, which can be derived after a number of significant simplifications and, as a result, allow for analytical solution.

As was mentioned above, the continuum-based model may not be valid for microdevices and there are a number of so-called particle-based models when a particle represents an average behaviour of many atoms. This allows us to employ them in these cases when the full atomistic models are not feasible as the number of atoms is too big even for microdevices but continuum-based models already fall short.

In order to make the application of the theory feasible, it is necessary to choose the right level of abstraction to be able to make simulation within given time limits and budget constraints. Also, an important question for any simulation is the reliability of results: to what extent one can believe in them. It is always necessary to verify the simulation algorithms and validate the original mathematical models. To this end, the simpler the model the better. As a result, a common sense approach is to choose the simplest model which can answer the engineering questions required.

Let us discuss the key questions for the development of the microthruster array, which have been specified after a number of discussions within the European project “Micropyros” and will be discussed in more details elsewhere.² For the present paper, they are taken as an input to the simulation group with the target to develop a modelling strategy.

Table 1: Hierarchy of models

Model	Input	Output	Example for the gas flow
Lumped or empirical representation	Device description and empirical parameters	Quantitative device behaviour	Ideal rocket theory
Continuum-based	Device description and material properties	Quantitative device behaviour	Navier-Stokes equations
Particle-based	Device description and empirical parameters	Quantitative device behaviour	Direct Simulation Monte Carlo
Atomistic: molecular dynamics or Monte-Carlo	Potential energy surface	Material properties	Determining viscosities, heat conductivities, reaction energies and rates
Quantum chemistry	n/a	Potential energy surface	n/a

It is necessary to choose:

- 1) a wafer material (silicon, ceramics, or glass) and a technology to manufacture it,
- 2) a technology for the low-temperature bonding of the wafers,
- 3) a solid fuel composition and a technology for its filling into mm square cavities,
- 4) a packaging technology,
- 5) a flight qualification procedure,

and then to develop:

- 1) the optimal geometrical design for the microthruster array,
- 2) an intelligent driving circuit to operate it.

Pragmatically, the goal of the Micropyros team is to search for an optimal combination between different available technologies in order to have a microthruster array producing impulse-bits as required for a minimum production cost. Hence, the simulation, in our view, should focus on the last two points, that is, to prepare the theory of operation of a microthruster and to choose the best approaches for its simulation from the viewpoint of the project goals. This will be considered in detail in the next sections.

Microthruster Theory of Operation

Microthruster functioning comprises at least an electro-thermal process, ignition, sustained combustion, membrane rupture and finally gas dynamics, and an engineer has to become an expert in all these areas in order to develop a successful device.

Electro-Thermal Process

A microthruster device is activated when the circuitry passes electrical power to a resistor. This produces heat within the resistor and leads to eventual heat transfer to the ignition material. The quantum level of electron and heat transfer^{10,11} cannot be reached in the microthruster. Thermal properties are available for most materials¹² and if necessary they can be measured experimentally or estimated from molecular simulation.¹³

Under a continuum-based approximation, the electrical part is described by the current continuity equation¹⁴

$$\nabla \cdot \mathbf{j} = 0 \quad (1)$$

where \mathbf{j} is the current density vector and it is supposed that there is no current source density within the resistor. For isotropic conductivity the constitutive relation is given by

$$\mathbf{j} = \sigma \nabla \psi \quad (2)$$

where σ is the conductivity for a given point and ψ is the electric potential. It is possible to solve Eqs (1)

and (2) for the unknown electric potential field provided the geometry of the resistor, its conductivity (or the resistivity) that may depend on temperature and the boundary conditions are specified.¹⁵ Note that Eqs (1) and (2) depend only implicitly on time due to a possible change in boundary values or a change in conductivity. This is because the speed of electron propagation is very high. We will assume that Eqs (1) and (2) hold instantly at any given time. A higher level model based on the solution of the electromagnetic Maxwell equations is required only if the frequency of the electrical current reaches the kHz range, i.e., when capacitance and inductive effects have to be accounted for.

The heat transfer from the resistor to the solid fuel is described by a heat conduction equation¹⁶

$$\nabla \cdot (\kappa \nabla T) + Q - \rho C_p \frac{\partial T}{\partial t} = 0 \quad (3)$$

where κ is the thermal conductivity (assumed to be isotropic), C_p is the specific heat capacity, ρ is the mass density, Q is the heat generation rate per volume (this term is non-zero within the resistor only) and T is the unknown temperature distribution that is to be determined over the device domain Ω with boundary Γ .

The coupling of Eqs (1) and (2) with Eq (3) is done by the Joule law for the heat generation rate per volume within the resistor

$$Q = \frac{j^2}{\sigma} \quad (4)$$

The equations above can be simplified under further assumptions. First, often it is possible to assume a lumped representation of the resistor, in other words, that the heat generation rate is homogeneous within the resistor, and to estimate it as

$$Q = I^2 R / V \quad (5)$$

where I is the total current going through the resistor, R its total resistance and V is its volume. This approximation de-couples Eqs (2) and (3). Next, if we assume that thermal material properties do not depend on temperature, the partial differential equation (3) becomes linear, which highly simplifies its solution. Finally, a 2D-axisymmetrical model can be employed as a first approximation to model the heat transfer within a particular microthruster.

In microsystem packaging, the Biot number is used to determine whether one can ignore a geometry of a spreader plate in order to model the heat transfer from a microchip to this plate.¹⁷ This cannot be directly applied to a microthruster, but analogous consideration shows that it is highly unlikely that in our case one can use a lumped approximation for Eq (2).

Ignition and Sustained Combustion

The heat of the resistor causes heating of the solid fuel. This, in turn, leads to its ignition and to the formation of sustained combustion. The solid fuel can be double-based (homogeneous) or composite (heterogeneous), and it contains both oxidizing and reducing agents.¹⁸ During sustained combustion, the heat produced in the flame propagates to the fuel and causes its decomposition. As a result, the overall phenomena is a thin, spontaneously moving front, the velocity of which is referred to as a burning rate.¹⁹ These phenomena are most difficult to model because one has to add chemistry, that is, reaction rates to conventional physical models, and the number of elementary reactions occurring during combustion may well reach into the hundreds.

If the thermodynamic properties of the fuel are known, it is possible to estimate the so-called adiabatic flame temperature and use it for rough estimates of maximum specific impulse.⁹ This is sometimes referred to as 0D (zero-dimensional) gas dynamics, because the computations are of the thermodynamic nature and are based on the original and final states only, and the transition between them does not appear explicitly within the formalism.²⁰

There are a number of approaches on the continuum level to treat the burning rate.²¹ The simplest models are based on Quasi-Steady gas phase, Homogeneous solid phase, One Dimensional (QSHOD) assumptions²² when all the reactions in the gas phase are modeled as a single overall reaction. In order to apply these theories, it is necessary to supply a number of empirical parameters specific to a particular solid fuel. Today, there is a tendency to develop models based on detailed chemical mechanisms of sustained combustion,^{23,24} but in order to use them it is necessary to know the rate constants for all the elementary processes under consideration. Rate constants are to be measured experimentally under specially prepared conditions or are estimated by means of molecular modelling.²⁵

On the other hand, there are many experimental observations on burning the solid fuel.^{18,21} In many cases, such results as the ignition and flame temperatures and the empirical burning rate can be used directly from experimental measurements as inputs to other models.

The results discussed above concerns big rockets and they may need to be modified for a microthruster. The heat exchange of the burning front with the surrounding chamber is usually ignored in macromodels for sustained combustion, and this is unacceptable for the microthruster. It has been demonstrated that, because of the heat losses, the burning rates measured at the macroscale are not applicable to chambers in the millimeter range.² An extreme example is the fact

that the common composite propellant made of hydroxyl-terminated polybutadiene (HTPB) with ammonium perchlorate (AP) oxidizer does not produce a sustained combustion in a small silicon chamber.⁴ Silicon's high thermal conductivity, coupled with the large area to volume ratio of the chamber, simply cools the reaction front too efficiently.

Membrane Rupture

The gas formation during ignition and sustained combustion increases the pressure within the microthruster chamber and this leads to membrane rupture. The membrane is needed to seal the chamber and is made up of brittle materials. In the membrane the tensile stress σ_x is approximately linearly proportional to the strain ϵ_x right up to rupture²⁶ and the Young modulus is effectively constant in this case.

The fracture of brittle materials is a stochastic process described well by a Weibull distribution. The membrane rupture occurs when, during the membrane deformation, the stress is close to the mean tensile strength, σ_f . This information might be used to simulate membrane rupture in the microthruster device by the finite element method. Typically in such simulations the membrane is modeled by so-called shell elements.²⁷ Because of high temperature semiconductor manufacturing process, the membrane dielectrics are prestressed at different stress intensities, and the shell elements need to take this into consideration.

For a quick estimation of the critical pressure within the microthruster device required to break the membrane, the theory of bulge testing^{28,29} could be employed. In this test the membrane film is sealed to the end of a hollow cylindrical tube, which in turn is pressurized with gas. This setup is very close to what is happening within the microthruster.

It should be noted that the results of both approaches depend on the material properties employed. Note that the tensile strength decreases when the temperature increases and this must be taken into account, for example by heating the resistor during the bulge test. This may mean that the experimental measurement of the critical pressure is easier to perform when compared with tensile strength determination followed by a simulation.

The scaling of mechanical properties is discussed in^{30,31} and there are a series of molecular simulations that shed additional insight on the fracture process.^{32,33}

Gas Dynamics

The continuum-based equations for fluid flow, the Navier-Stokes equations, describe the conservation of mass, momentum and energy.^{34,35} They are based on an assumption that the molecular velocity distribution of the flow is close to the Maxwell distribution. This is

valid when the molecular mean free path is much less than the characteristic dimension of the system, in other words, for small Knudsen numbers. The Knudsen number of the flow increases when the pressure or the size of the system decreases. For flows with a Knudsen number greater than 0.001, one may correct the Navier-Stokes equations by introducing slip boundary conditions, and then for even larger Knudsen numbers it is necessary to switch to the solution of the Boltzmann equation or to molecular dynamics simulation. As full-scale atomistic simulations are unfeasible for micronozzles, the so-called Direct Simulation Monte Carlo method^{36,37} enjoys widespread use here.

A solution of the Navier-Stokes equations in the general case for arbitrary 3D geometry is still a formidable computational task. If one neglects gravity (an external force) and the viscosity and assumes that the velocity projection on the plane perpendicular to the nozzle axis is small when compared to its projection on the nozzle axis, then this leads to an effectively one-dimensional problem (quasi-1D flow)³⁵ as follows

$$\frac{\partial(\rho S)}{\partial t} + \frac{\partial(\rho u S)}{\partial x} = 0 \quad (6)$$

$$\frac{\partial(\rho u S)}{\partial t} + \frac{\partial[(\rho u^2 + p)S]}{\partial x} = p \frac{dS}{dx} \quad (7)$$

$$\frac{\partial(\rho e S)}{\partial t} + \frac{\partial(\rho u h S)}{\partial x} = q \quad (8)$$

where ρ is the density, u is a projection of the velocity on the nozzle axis, S is a cross-section of the nozzle, p is the pressure, e is the specific energy, h is the enthalpy and q is a total heat exchange with the nozzle for a given cross section.

In rocket science, thrust and impulse conventionally are estimated using the concept of a so-called ideal rocket.⁹ This corresponds to the stationary solution of the quasi-1D flow after neglecting a source term on the right side and under the assumption of the equation of state for a perfect gas. The resulting system has an analytic solution that is analogous to the lumped representation in MEMS.

The equations for the “ideal rocket” require knowledge of the pressure in the nozzle chamber. In the case of burning of the solid fuel, it can be found from the mass conservation equation in the form⁹

$$A_b r \rho_b = \frac{d}{dt}(\rho_1 V_1) + A_1 p_1 \sqrt{\frac{k}{RT_1} \left(\frac{2}{k+1}\right)^{(k+1)/(k-1)}} \quad (9)$$

where r is the burning rate of the solid fuel, A_b is the burning area of the solid fuel, ρ_b is the density of the solid fuel, ρ_1 is the density of the gas in the nozzle chamber, T_1 and V_1 are its temperature and volume.

Eq (9) is based on the assumption that the relaxation of the gas flow is much faster than the velocity of the moving front of the burning fuel. As a result, it uses a stationary solution for the gas dynamics described above and rudimentary kinetics to take into account a change in the volume of the nozzle chamber because of the moving burning front of the solid fuel.

An important choice in all fluid dynamics models is a realistic model for describing the gas phase, because it might influence all the properties of the gas flow considerably. In our case during sustained combustion, we have not an ideal gas but rather a reactive flow. This means that the gas phase consists of a number of species and they interact with each other.³⁸ Here one can choose between a kinetic approach, which is more realistic, or a thermodynamic one under the local equilibrium hypothesis, which is computationally much faster.

It is important to estimate the heat transfer between the gas flow and the surrounding wafer. In principle, this can be done by including the heat transfer into the Navier-Stokes equations or by the Direct Simulation Monte Carlo method. Nevertheless, reasonable results can be obtained by means of an approximate equation in the form⁹

$$q = h(T_b - T_s) \quad (10)$$

where q is the heat transferred per unit area per unit time, T_b is the bulk temperature in the gas phase, T_s is the temperature at the surface of the wafer, and h is the gas film coefficient, describing the heat transfer through the boundary layer. This corresponds to a convection boundary condition in heat transfer methods and can easily be added there. The gas film coefficient can be estimated from the Nusselt number, which in turn is related to the Reynolds and Prandtl numbers by several correlation equations.^{9,39}

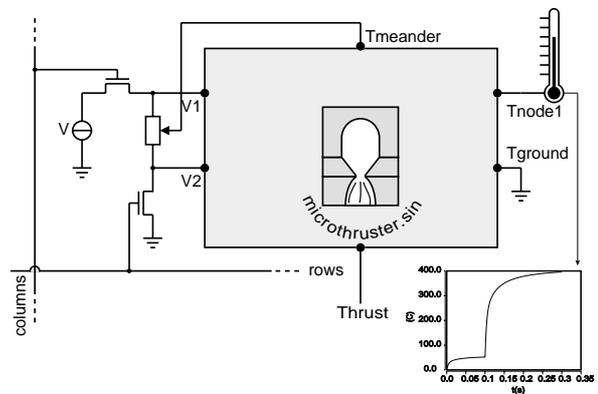


Fig. 2. Compact model of the microthruster to allow for a joint simulation: the electrical current heats up the resistor that causes fuel ignition, leads to sustained combustion and finally produces the desired impulse.

Table 2: Models for the microthruster operation

Task	Available models	Modelling strategy
Electro-thermal ignition	<ol style="list-style-type: none"> 1) Coupled Poisson and heat transfer equations, Eqs (1) to (4). 2) Lumped resistor and heat transfer, Eqs (3) and (5). 3) Lumped heat transfer. 	The lumped resistor and 3D heat transfer model discretized with the finite element method and followed by a model order reduction.
Ignition and sustained combustion	<ol style="list-style-type: none"> 1) Detailed chemical kinetics. 2) QSHOD. 3) Adiabatic flame temperature. 	Experimental ignition temperature as input to the electro-thermal ignition problem, experimental burning rate and flame properties as inputs to gas dynamics.
Membrane rupture	<ol style="list-style-type: none"> 1) Molecular and multiscale simulations. 2) Finite element method. 3) Bulge test theory. 	Bulge test model and experiments.
Gas dynamics	<ol style="list-style-type: none"> 1) Direct Simulation Monte-Carlo. 2) Navier-Stokes equations for the reactive flow. 3) Local equilibria hypothesis to treat chemistry. 4) Fixing chemical composition at the flame front. 5) Quasi-1D approximation. 6) Ideal rocket model. 	Ideal rocket model followed by empirical corrections.

Recommended Model

As was already mentioned, the modelling goal is to help to choose the optimal geometry to fabricate the microthruster array as well as to develop an intelligent electrical circuit, schematically shown in Fig. 2. Let us start by listing the most important challenges for technologists and engineers here.

The final output desired is clearly the same as for big rockets: a given impulse produced by a microthruster. The optimization of the nozzle shape plays an important role in conventional rockets.⁹ Nevertheless, this can be hardly applied to the microthruster array, because in the case of the geometry shown in Fig. 1 the technological degrees of freedom for the nozzle optimization are very limited. In the current design, it is only possible to change slightly the diverging angle in the nozzle wafer, and one cannot even think of an optimal nozzle shape design. As usual, it is possible in principle, but for production cost outside of any serious consideration, because the nozzle is in a direction perpendicular to the silicon wafer surface.

From a technological point of view, the disadvantage of non-optimal impulse production by an individual microthruster can be overcome by a higher integration of microthrusters on a chip. The main

question here is rather unusual for conventional rocket science, that is, to predict the highest possible level of integration of microthrusters on a chip. A high level of integration can be achieved by reducing the size of a microthruster and by placing microthrusters closer to each other. The lower limit on microthruster size comes from the fact that, because of the heat losses, conventional solid fuels do not display sustained combustion when the diameter is too small.^{2,4} The limit on the distance between microthrusters is determined by thermal crosstalk. Hence, heat management becomes one of the main goals for microthruster simulation as it is necessary to thermally isolate neighboring microthrusters.

In the current project, the goal is to use available compositions of solid fuel and, as a result, the modelling strategy is to bear upon experimentally determined fuel properties such as ignition temperature, burning rate, and flame temperature for a given chamber. The problem of the optimization of the solid fuel composition specifically for a microthruster array with a given diameter of the chamber and the heat conductivity of the wafer is left for future research. The main emphasis is made on predicting and managing the heat flow.

There are two sources of heat that lead to the thermal crosstalk. First is the heat, which is governed by the driving circuitry, from the resistor to the solid fuel, and second is the heat transfer from the hot gases to the wafer during the gas dynamics phase. There are many engineering degrees of freedom to influence this: a position and shape of the resistor, the introduction of special grooves between microthrusters and so on.

Other degrees of freedom are tied with the driving circuitry. In the first phase, the circuitry has all means to completely control the resistor heating because it can directly measure the nonlinear resistor's temperature. After the onset of ignition, the circuit loses control and subsequent steps happen automatically. The circuit can influence sustained combustion indirectly only by means of preheating of the solid fuel before ignition as the burning rate depends on the fuel temperature. This gives a natural way to de-couple the simulation of the whole process: electro-thermal process which should reach the ignition temperature and the gas dynamics when the fuel characteristics will be used as input parameters.

To conclude, at the current level of development, the model for a microthruster array must include an involved electro-thermal simulation and to be able to make a joint simulation of the array simultaneously with the driving circuitry. In our view, all other aspects of microthruster operation can be modeled just on a basic level. Oddly enough, the development of the microthruster array happens to be closer to microsystem packaging¹⁷ than to rocket science. The recommended models are summarized in Table 2.

Model Reduction

As was discussed in section "Electro-Thermal Process", Eq (3) cannot be simplified but rather it is necessary to solve it with Eq (5) for a given 3D geometry. This is done by the finite element method that, after discretization but before actually solving, produces a system of first order ordinary differential equations (ODEs)

$$\begin{cases} G \cdot \frac{dT}{dt} = A \cdot T + bI^2R/V \\ y = C \cdot T \end{cases} \quad (11)$$

where the vector T contains all unknown nodal temperatures on a grid to be found and the vector y contains several outputs, which actually should be determined. A , C and G are matrices, and b is the vector coupling input from the electrical circuit via Eq (5).

In general, Eq (11) is nonlinear because the material properties depend on temperature and thus the system matrices are not constant. Fortunately, this nonlinear-

ity is relatively weak and quite an appropriate strategy is to linearize the system around an operation point. The only exception is the dependence of resistivity on temperature, because it is important to leave it to allow the circuitry to measure the temperature. Yet, under the assumption of the homogeneous heat rate within the resistor expressed by Eq (5), it is still possible to have system matrices constant because the total resistivity is included in the input function from the electrical circuit only.

The dimensionality of the state vector T in Eq (11) is very high, in the case of 3D finite element simulation it can easily reach hundreds of thousands. If it is necessary to solve it just once then this may not be a problem, however this, without doubt, prevents a joint electro-thermal simulation of hundreds of thrusters with their driving circuitry.

This problem expressed by Eqs (3), (5) and (11) is very important for packaging of microsystems. In a way, the successful work of a microthruster array and a microscheme is very similar as they both depend on the right thermal management. The difference is tied with the goal: for a microthruster to reach critical temperature, for a power transistor not to reach it. From the simulation viewpoint, they are very similar. In packaging, there are approaches to obtain "compact" thermal models for a system level simulation,^{17,40} that is, to reduce significantly the dimension of the state vector T in Eq (11). After all, engineers are not interested in the whole temperature field but in a few temperatures in the most important parts of the device. Unfortunately, the packaging community develops compact models based on engineering intuition and is apparently not aware of the advanced mathematical methods for model order reduction⁴¹ (see Table 3) which allows us to represent the large order dynamic system (11) with high level of accuracy by a low order system

$$\begin{cases} \hat{G} \cdot \frac{dz}{dt} = \hat{A} \cdot z + \hat{b}I^2R/V \\ y = \hat{C} \cdot z \end{cases} \quad (12)$$

where z is a reduced state vector and the "hat" symbol marks the reduced system matrices.

Based on the review,⁴¹ we have chosen a moment matching technique built upon an Arnoldi process as a basis for the model reduction to be used in Micropyros and demonstrated that it works quite well for our case.⁴²

Conclusion

A microthruster array model must combine electrical circuit, heat transfer, combustion and gas dynamics. It must take into consideration the effects of miniaturization on the one hand and massive parallel-

ism (hundreds of thrusters) on the other. In this paper we have outlined the models, their limitations, and available solution methods. Finally, we have described a strategy which will render the models computationally tractable and hence practically applicable.

Acknowledgments

This work is partially funded by the EU through the

project MICROPYROS (IST-1999-29047), partially by the DFG project MST-Compact (KO-1883/6) and partially by an operating grant of the University of Freiburg.

We appreciate very useful discussions with our partners in the MICROPYROS project.

Table 3: Methods of model reduction of linear dynamics systems

Name	Advantages	Disadvantages
Control theory (Truncated Balanced Approximation, Singular Perturbation Approximation, Hankel-Norm Approximation)	Have a global error estimate, can be used in a fully automatic manner.	Computational complexity is $O(N^3)$, can be used for systems with order less than a few thousand unknowns.
Padé approximants (moment matching) via Krylov subspaces by means of either the Arnoldi or Lanczos process.	Very advantageous computationally, can be applied to very high-dimensional 1st order linear systems.	Does not have a global error estimate. It is necessary to select the order of the reduced system manually.
SVD-Krylov (low-rank Gramian approximants).	Have a global error estimate and the computational complexity is less than $O(N^2)$.	Just under development.

References

- [1] C. Rossi, *Micropropulsion for Space - A Survey of MEMS-based Micro Thrusters and their Solid Propellant Technology*, Sensors Updates, 2002, 10, 257-292.
- [2] B. Larangot, T. Camps, A. Berthold, C. Rossi, D. Estève, P. Q. Pham, D. Briand, N. F. de Rooij, M. Puig-Vidal, P. Miribel, E. Montané, G. Macías, J. Samitier, *Solid Propellant Micro rockets - Towards a New Type of Power MEMS*, Nanotech'02, 2002, AIAA paper.
- [3] D. H. Lewis, S. W. Janson, R. B. Cohen, E. K. Antonsson, *Digital micropropulsion*, Sens. Actuator A-Phys., 2000, 80, 143-154.
- [4] D. Teasdale, V. Milanovic, P. Chang, K. S. J. Pister, *Microrockets for Smart Dust*, Smart Mater. Struct., 2001, 10, 1145-1155.
- [5] M. T. Heath, W. A. Dick, *Virtual prototyping of solid propellant rockets*, Comput. Sci. Eng., 2000, 2, 21-32.
- [6] M. Gad-el-Hak, *The fluid mechanics of microdevices - The Freeman Scholar Lecture*, J. Fluids Eng.-Trans. ASME, 1999, 121, 5-33.
- [7] M. Parrinello, *Simulating complex systems without adjustable parameters*, Comput. Sci. Eng., 2000, 2, 22-27.
- [8] A. R. Leach, *Molecular Modelling: Principles and Applications*, second edition, Pearson Education EMA, 2001.
- [9] G. P. Sutton, O. Biblarz, *Rocket propulsion elements*, 7th ed, New York: John Wiley & Sons, 2001, 751 p.
- [10] A. Greiner, L. Reggiani, T. Kuhn, L. Varani, *Thermal conductivity and Lorenz number for one-dimensional ballistic transport*, Phys. Rev. Lett., 1997, 78, 1114-1117.
- [11] L. G. C. Rego, G. Kirzenow, *Quantized thermal conductance of dielectric quantum wires*, Phys. Rev. Lett., 1998, 81, 232-235.
- [12] *CRC handbook of chemistry and physics: a ready-reference book of chemical and physical data*, Chemical Rubber Company, Boca Raton, 1999.
- [13] D. Frenkel and B. Smit, *Understanding Molecular Simulation*, Academic Press, San Diego, 1996.
- [14] A. Nathan, H. Baltes, *Microtransducer CAD: physical and computational aspects*. Wien; New York: Springer, 1999, 427 pp.
- [15] J. G. Korvink, H. Baltes, *Microsystem Modeling*, Sensors Update, 1996, 2, 181-209.
- [16] H. H. Huang, A. S. Usmani, *Finite Element Analysis for Heat Transfer*, Springer-Verlag London, 1994.
- [17] W. Nakayama, *Thermal issues in microsystems packaging*, IEEE Trans. Adv. Pack., 2000, 23, 602-607.
- [18] N. Kubota, *Propellants and Explosives: Thermochemical Aspect of Combustion*, John Wiley & Sons, 2001.

- [19] F. A. Williams, M. Barrère, N. C. Huang, *Fundamental aspects of solid propellant rockets*, AGARDograph no. 116, Slough, London, Published for the Advisory Group for Aerospace Research and Development of N.A.T.O. by Technivision Services. 1969, 791 pp.
- [20] C. E. Baukal, V. Y. Gershtein, X. Li, *Computational fluid dynamics in industrial combustion*. Boca Raton: CRC Press. 2001, 630 pp.
- [21] *Solid propellant chemistry, combustion, and motor interior ballistics*. Progress in astronautics and aeronautics, ed.: V. Yang, T. B. Brill, W.-Z. Ren: American Institute of Aeronautics and Astronautics. 2000, v. 185, 990 pp.
- [22] M. Q. Brewster, *Solid Propellant Combustion Response: Quasi-Steady (QSHOD) Theory Development and Validation*, in ²¹, p. 607-637.
- [23] Y. C. Liau, V. Yang, S. T. Thynell, *Modeling of RDX/GAP Propellant Combustion with Detailed Chemical Kinetics*, in ²¹, p. 477-500.
- [24] M. S. Miller, W. R. Anderson, *Energetic-Material Combustion Modeling with Elementary Gas-Phase Reactions: A Practical Approach*, in ²¹, p. 501-531.
- [25] D. Chakraborty, M. C. Lin, *Gas Phase Chemical Kinetics of [C,H,N,O] Systems Relevant to the Combustion of Nitramines*, in ²¹, p. 33-71.
- [26] W.D. Callister, *Materials science and engineering: an introduction*, New York; Weinheim: Wiley, 2000.
- [27] T. Belytschko, W.K. Liu, B. Moran, *Finite Elements for Nonlinear Continua and Structures*, Wiley, 2000.
- [28] M. Ohring, *The materials science of thin films*, Boston: Academic Press, 1992.
- [29] O. Kraft, C.A. Volkert, *Mechanical testing of thin films and small structures*, Adv. Eng. Mater., 2001, v. 3, N. 3, p. 99-110.
- [30] E. Arzt, *Size effects in materials due to microstructural and dimensional constraints: A comparative review*, Acta Mater., 1998, 46, 5611-5626.
- [31] S. M. Spearing, *Materials issues in microelectromechanical systems (MEMS)*, Acta Mater., 2000, 48, 179-196.
- [32] H. Rafii-Tabar, *Modelling the nano-scale phenomena in condensed matter physics via computer-based numerical simulations*, Phys. Rep.-Rev. Sec. Phys. Lett., 2000, 325, 240-310.
- [33] A. Nakano, M. E. Bachlechner, R. K. Kalia, E. Lidorikis, P. Vashishta, G. Z. Voyiadjis, T. J. Campbell, S. Ogata, F. Shimojo, *Multiscale simulation of nanosystems*, Comput. Sci. Eng., 2001, 3, 56-66.
- [34] C. A. J. Fletcher, *Computational techniques for fluid dynamics*, Berlin; Heidelberg: Springer, (Springer series in computational physics), 1991.
- [35] C. Hirsch, *Numerical computation of internal and external flows*, Chichester: Wiley; (Wiley series in numerical methods in engineering), 1992.
- [36] G. A. Bird, *Molecular gas dynamics and the direct simulation of gas flows*, Oxford: Clarendon, 1994, 458 p.
- [37] E. S. Oran, C. K. Oh, B. Z. Cybyk, *Direct simulation Monte Carlo: Recent advances and applications*, Annu. Rev. Fluid Mech., 1998, 30, 403-441.
- [38] V. Giovangigli, *Multicomponent flow modeling*, Boston; Basel; Berlin: Birkhäuser, (Modeling and simulation in science, engineering and technology), 1999.
- [39] R. A. Ahmad, *Discharge coefficients and heat transfer for axisymmetric supersonic nozzles*, Heat Transf. Eng., 2001, 22, 40-61.
- [40] C. S. Yun, P. Malberti, M. Ciappa, W. Fichtner, *Thermal Component Model for Electrothermal Analysis of IGBT Module Systems*, IEEE Trans. Adv. Pack., 2001, 24, 401-406.
- [41] E. B. Rudnyi, J. G. Korvink, *Automatic Model Reduction for Transient Simulation of MEMS-based Devices*, Sensors Update, 2002, 11, to appear.
- [42] T. Bechtold, E. B. Rudnyi, J. G. Korvink, *Automatic Order Reduction of Thermo-Electric Model for Microthruster Ignition Unit*, Proc. of International Conference on Simulation of Semiconductor Processes and Devices (SIS-PAD), 2002.