

A Simple Atomic Scheme for Ar Thruster Multidimensional Modeling and Optical Diagnostics

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Abstract: Optical diagnostics and modeling of plasma thrusters fed with Ar can be obtained using a “zero dimension” Collisional-Radiative model in conjunction with a multi-dimensional model taking account of the species transport. We report on detailed evaluation of the necessary atomic parameters which allows to study and optimize various space applications in presence of Ar plasma.

Nomenclature

3,4CTMC	=	three, four body classical trajectory Monte Carlo codes
$A_{i,j}$	=	transition probability, level j to i
ACE	=	atomic collisions with electrons code
Ar I, II,..	=	successive spectra of the argon homo-nuclear sequence
Ar/C-R	=	multi-stage collisional – radiative model for Argon plasmas
ArI,II/C-R	=	collisional – radiative model containing only 4 lines of Ar I and 5 of Ar II and their continua
Ar/GI	=	Global kinetic models for Ar plasma (as simplified EIRENE, Stookes, commercial ...)
CATS	=	Cowan atomic structure code
CbA	=	Coulomb approximation code
C-R	=	collisional – radiative model
CO	=	coronal model
DW	=	distorted wave approximation
EIRENE	=	particle transport code
FOMBT	=	first order many body theory
GL	=	ground level compound, composed by one sole level for Ar I, two for Ar II, five for Ar III
j_c	=	total angular momentum of the core
jK/LS	=	coupling schemes
l	=	orbital quantum number, $s = 0, p = 1, d = 2, f = 3, \dots$
LANL	=	Los Alamos National Laboratory
LHS	=	left hand side of the equation
LTE	=	local thermodynamic equilibrium

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n	= principal quantum number, here $n = 3, 4$
NIST	= National Institute of Standards and Technology, Gaithersburg (USA)
PIC	= Particle in Cell type code
RDW	= relativistic distorted wave approximation
RHS	= right hand side of the equation
SPT-50	= prototype stationary plasma thrusters, 50 mm of diameter
SST	= SUPERSTRUCTURE code
T_e	= electronic temperature
UV	= ultraviolet spectral region
Ar I, II,..	= successive spectra of the argon homo-nuclear sequence
σ_e^E	= electron collision excitation cross section
σ_e^I	= electron collision ionization cross section

I. Introduction

ATOMIC data are important for the optical diagnostics of Ar fed plasma thrusters and, more generally, for the study of experimental, natural and industrial plasmas. Typically, the plasmas encountered in electric propulsion are not in Local Thermodynamic Equilibrium (LTE), therefore a huge amount of atomic data must be used, which describe the plasma properties in each point by a “zero dimension” Collisional-Radiative (C-R) model. This model takes account of the main collisional and radiative processes by means of the corresponding transition probabilities and cross sections integrated over the prevailing distributions, often taken as maxwellian. Atomic data are entering the RHS of the statistical equations constituting the C-R model¹. “Zero dimension” refers to the fact that the level populations expressed by the C-R model and obtained by resolving locally the set of the statistical equations are only valid in the considered point. Transport of the species is generally neglected in the C-R models, an approximation valid only for homogeneous plasmas. Moreover, in case that each of the LHS of the statistical equations is set to zero the code is valid only for stationary plasmas. It is possible to take into account the transport of all the present ion species by an adjoint transport code, which takes care of the particle transfer. We have proposed previously² to use the EIRENE code³ for this purpose. This code is developed at the ‘Institut für Plasmaphysik’, Jülich, mainly for modeling Tokamak plasmas and includes in general the kinetics of any species present in the plasma as atoms and molecules and their ions. It so constitutes a type of integrated numerical experiment including plasma physics, atomic and molecular processes and plasma-wall interaction. Although we are in the process of implementing some of our atomic models into this code, we are also considering using of simplified codes of Hydrodynamic, Particle in Cell (PIC) or Hybrid type, together with a C-R model containing a reduced number of ionization stages and excited levels, valid whenever the electronic temperature T_e is sufficiently low. In order to drastically reduce the computational effort in such a scheme, we have to keep the total number of the considered levels to a strict minimum. Such a global model can be useful in studying electric propulsion, reentrance and plasma reactors. In the field of C-R modeling and diagnostics of plasma thrusters fed with Ar, our previously developed C-R model Ar/C-R was applied in the past to the study of one SPT-50 prototype device⁴ which was made available to us in the LPP Laboratory of the Polytechnic school at Palaiseau. This prototype was occasionally fed with an Ar-Xe mixture and with pure Ar and diagnosed in the latter case by our Ar/C-R model, which initially contained only the Ar I, II and III spectra⁵. It has been thoroughly validated by comparison with various experimental spectra. Here we specifically address electric propulsion using Ar fuelling in case the temperature is sufficiently low to justify consideration of Ar I and Ar II spectra only, with the Ar III spectrum reduced to its ground level. We have developed a simplified C-R model based in averaged states to be used with the global models valid in such conditions. This simplified model (ArI,II/C-R) constitutes a significant simplification of our previous Ar plasma C-R model (Ar/C-R) used for the optical diagnostics of the SPT-50 prototype, both in the number of the considered ionization stages and in the number of the contained excited states, which are here all averaged and pertain only to lowly excited species.

ArI,II/C-R has been developed to obtain a necessary simplification of the description of the atomic characteristics of the plasma constituents, but it contributes also in the optical diagnostics of the modeled plasma: It suffices to share the total population of each averaged level calculated by the ArI,II/C-R model following our full Ar/C-R model results, in order to infer the theoretical intensities of the observed real transitions needed for the optical diagnostics.

We give a brief description of various modeling codes in Chap. II of the paper. Evaluation and validation of the necessary atomic data are presented in Chap. III. Description of the optical diagnostics and conclusion are given thereafter in Chaps. IV and V correspondingly.

II. General Characteristics of the Models

Detailed diagnostics and modeling of relatively low energy Ar plasmas of interest to propulsion, re-entry plasma simulations and similar cases call first for a C-R model taking into account at least the ground levels of the Ar I and Ar II species and their lower excited states. Depending on the application, the Ar III ground state and its excited states could also appear if necessary. A decision on the upper limit choice can be made on the basis of a simplified Coronal (CO) model and/or following the emission spectra registered experimentally for each case. As was explained elsewhere¹, solution of the complete set of the non-stationary statistical equations with non-zero LHS part cannot be considered. Moreover, evaluation of the macroscopic coefficients entering in the RHS of the system equations on the basis of the corresponding microscopic cross sections is hampered whenever the distributions deviate from Maxwellian. Therefore, only the most populated states are to be retained. Furthermore, a realistic modeling taking into account the plasma geometry, the kinetics of the species including the possibly existing instabilities, calls for a complementary multidimensional kinetic model, in which, as a first approximation, we introduce only the essential features of the atomic structure. This can be made e.g. by using an averaged level to represent collectively a whole multiplet, instead of its fine structure components. In the following, we review briefly the main characteristics of the various model types, which may contribute separately or simultaneously to the plasma diagnostics and modeling.

A. The Ar C-R Model

It is well known that a multi-stage C-R model is necessary for a satisfactory non-LTE plasma diagnostics. Such a model (Ar/C-R) has been previously developed and validated⁶. It describes the spectra of lowly ionized Ar species (Ar I, II, III etc) according to the application needs. As we are considering here only low energy plasmas, taking into account of the two first species Ar I and Ar II with its continuum, i.e. the Ar III ground level, is enough for the analysis of the main part of the spectra expected to be registered in a prototype thruster fed with Ar. The complete Ar I, II and III low energy spectrum has been previously analyzed⁷, in order to validate such a C-R model.

B. A Simplified Model of the Ar I, II Structure

In order to keep the computational difficulties of a global model in a easily manageable level, we have developed a simplified C-R model based in averaged states to be used as an atomic structure skeleton for multidimensional global models valid in relatively low energies. A diagram for such a model (ArI,II/C-R) is given in Fig. 1, where arrows show only allowed transitions. Note that the numerous collisional excitation and ionization processes between the presented states are not shown in the figure. Averaged states of metastable and transitory character are noted by m and t correspondingly. Averaged energies of the proposed states are given in cm^{-1} . The total statistical weight for each state is given in parenthesis. This diagram includes only the most important configurations of the Ar I and Ar II spectra. Each of the Ar I and Ar II continua is put in a sole effective ground state, instead of the two and five real ones. The averaged excited states selected for the Ar I and Ar II spectra are not the same: In the Ar I case there is two distinguished real metastable and two resonant 4s levels, here averaged separately even if they belong to two different atomic cores ($^2P_{3/2}$, $^2P_{1/2}$). As for the Ar II, because the 4p levels are in general located higher than the 3d ones (there is even 4s levels located higher than the 3d, a fine structure detail not shown in Fig. 1), the meaning of metastable is

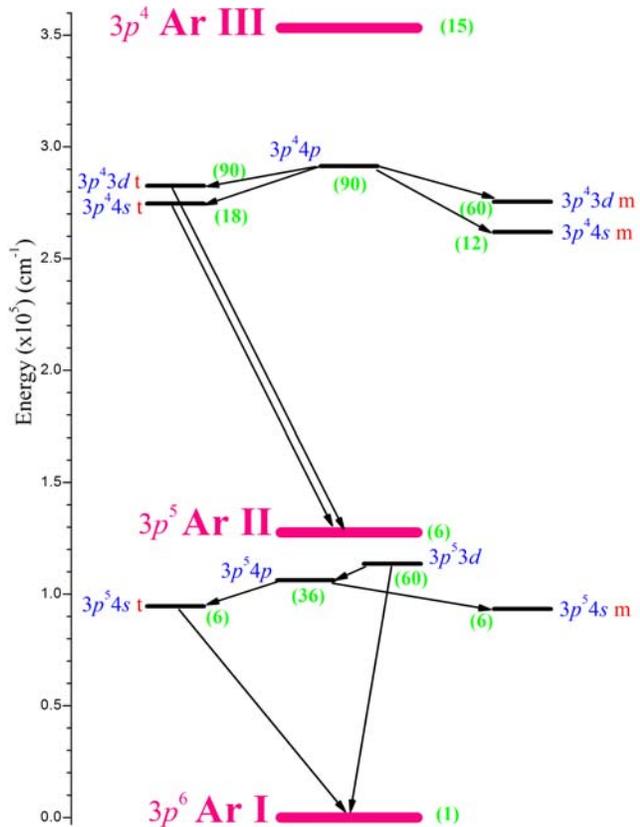


Figure 1. Simplified Grotrian diagram of the Ar I, II

somewhat biased. Accordingly, $3d$ levels have been also split here in a metastable and a transitory part, without distinction between the prevailing five cores. It is to be noted that higher excited levels and the whole Ar III spectrum, which become more important in higher temperatures, are neglected in the present model. Thusly we are left with only a dozen of averaged levels, accounting for more than thirty fine structure real levels, which are all present in Ar/C-R.

C. Global Plasma Models

As it was mentioned in the Introduction, the C-R models, valid for a sole point of the plasma, cannot take into account the description of the plasma as a whole. Such an effort has to be tackled by “global” models, which are noted here Ar/GI for the case of the Argon plasma modeling. Besides the aforementioned detailed EIRENE code, there is a multitude of such codes, more or less simplified, taking into account the global plasma properties related to the plasma geometry and stability and its interaction with the vessel walls if any. We have used previously such codes e.g. in the case of the dusty plasma modeling⁸, in an arc-jet study⁹ and in reentry plasma simulations¹⁰. Attention was paid in these cases to take correctly account of the essentials of the Ar atoms and ions structure, using simplified C-R models of the ArI,II/C-R type. Note that commercial packages containing general-purpose models may also be used as a tool for Ar/GI modeling.

In general, when constituting a C-R model, microscopic atomic data for each process are traditionally entering the RHS of the statistical equations under macroscopic form, after integration over a Maxwellian distribution. Nevertheless, for the present modeling needs, it is not sufficient to obtain a parametric form of the rates of interest. In fact, the species distributions are not taken as Maxwellian in the various Ar/GI codes but evaluated in each step of the calculation instead. Consequently, the cross sections are to be introduced in the codes, rather than the rates calculated with *ab initio* distributions as Maxwellian(s), Druyvesteyn, etc.

It is evident that the exclusive use of mean levels in the ArI,II/C-R model to replace the multiplet components prevent a direct optical diagnostics, as the theoretical lines, corresponding here to averaged levels, cannot be related directly with the lines appearing in the spectra. However, using a complete C-R model in conjunction, allows for optical diagnostics of the plasma and for validation of the global model: The values measured for the principal experimental lines of each multiplet can be compared to the corresponding theoretical values of the C-R model and their mean values are giving experimental values to compare with those corresponding to the mean levels values coming from the global model.

III. Evaluation of the Atomic Data

Among the needed atomic data, transition probabilities, electron impact excitation, ionization and photoionization cross sections are the most important. The last of them have been only used for calculation of the corresponding radiative recombination cross sections, the photon absorption being here negligible. Common theoretical codes have been used throughout for evaluation of most atomic data, because of the important lacks in the available experimental data⁷. In order to obtain recommended values for the needed data, we have made extensive calculations and evaluations in addition to previous detailed evaluations¹¹⁻¹⁵ of both the transition probabilities (A_{ij}) and of electron collision excitation cross sections (σ_{e}^E) concerning the excited levels of the $4s$, $4p/5p$ and $3d$ configurations of Ar I. Generation of the cross sections for ionization and recombination processes, allowing for the determination of the dynamic equilibrium between the ionization stages included in the model and also for other processes taking into consideration, was carried out as summarized elsewhere¹⁶.

A. Atomic Structure and Transition Probabilities of Ar I, II

For both the Ar I and Ar II evaluations of A_{ij} , results of calculations by CbA, a code developed previously by one of us (K.K.) and based in the well-known Coulomb Approximation¹⁷ have been extensively used. This code calculates the A_{ij} in the jK and in the LS coupling schemes. The jK coupling calculations lead to better results for Ar I than the LS ones, thus confirming our previous conjecture that the neutral rare gases Ne, Ar, Kr and Xe are better described in the jK coupling scheme. Data from CbA code were systematically compared with intermediate coupling results from the SUPERSTRUCTURE (SST) programme¹⁸ and from CATS, a code by R.D. Cowan as adapted for using it in the WEB¹⁹. Results of these calculations were compared with existing experimental measurements and with the values provided by NIST²⁰.

Especially for the Ar I case, a number of extensive previous evaluations^{21,22} of transition probabilities was already available. To support our present evaluations, Ar I and Ar II spectra have been recently studied experimentally⁶ in collaboration with the University of Ioannina and compared to previous experimental results²³.

B. Electron Collision Ionization

Ionization of atoms and ions by electron collisions in low temperature plasma is the essential mechanism for its ionization equilibrium. Consequently, numerous codes have been developed following various approximations for calculating the electron collision ionization cross sections (σ_e^I) of the Ar and its ions. A review of the σ_e^I calculations of most rare gas species with emphasis to R-matrix calculations was presented very recently²⁴. Experimental studies are also available. For the needs of the present simplified Ar model, we have used a very simple semi-empirical formula²⁵ adapted to the case of the lower Ar I and Ar II levels ionization according to the results of a few body problem code²⁶.

C. Electron Collision Excitation and De-excitation

Spontaneous emission and inelastic electron collisions are the two most important processes, not only for modeling purposes, but also because they define essentially the line intensities in the plasma spectra, which are necessary for diagnosing the plasma and validating the models. Further to our recent σ_e^E evaluations^{11,12}, we proceeded lately to additional evaluations¹³⁻¹⁵ of σ_e^E for the main Ar I configurations, based in existing experimental and theoretical data and also in calculations based in few body problem quasi-classical calculations, DW approximation calculations and semi-empirical formulas. Part of this work was presented recently elsewhere²⁷. We also work in improving the σ_e^E database pertaining to the main Ar II multiplets.

In order to get an idea of the cross section values, the global excitation rate curves for the $4s$ and $4p$ levels for a Maxwellian distribution, are given in Figs. 2 and 3. The corresponding values contained in the second edition of the book by Lieberman and Lichtenberg²⁸ are also shown in these figures for comparison. These authors recommend using of the provided parametrized curves only for low energies. This recommendation is justified by simple inspection of the Figs. 2 and 3. For a higher energy region (energies higher than ~ 30 eV) we use the values shown in the figures, obtained by our evaluations.

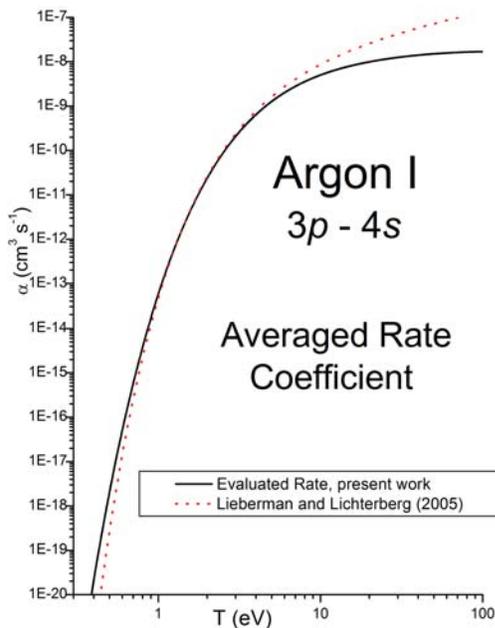


Figure 2. Average rate coefficient for $3p - 4s$

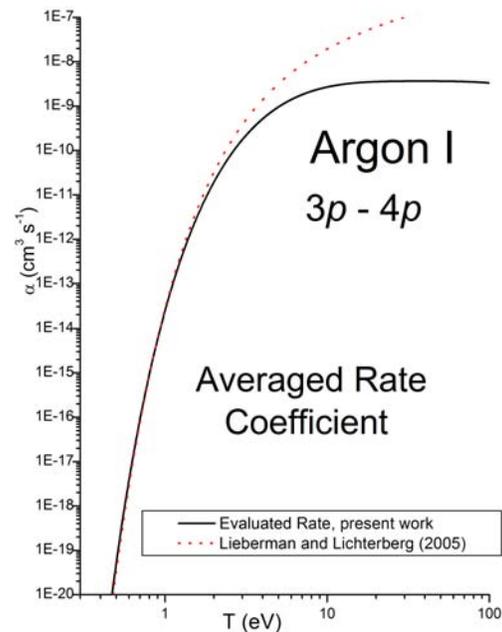


Figure 3. Average rate coefficient for $3p - 4p$

The partial σ_e^E involving each level of the $4s$ and $4p$ configurations were evaluated separately with codes using various types of approximations like these given by the ACE code (DW and FOMBT approximations) available by LANL, the well-known Born approximation, and the results of the relativistic RDW code. The so obtained values were compared with the existing experimental results and quasi-classical formulas. The latter were proposed previously²⁵ and extended on the basis of 3,4CTMC calculations²⁶.

De-excitation cross sections were evaluated from the corresponding σ_e^E curves by using the detailed balance principle.

D. Other Important Atomic Processes

Additional processes can be introduced in the code, depending on the plasma conditions. The most important of them are photo-ionization and radiative recombination, its inverse process. In fact, the first of them is of no importance for the present studies and are evaluated for the sole purpose to calculate the cross sections of the second, which essentially insures the equilibrium with the ionization cross section for each species.

IV. Optical Diagnostics

As explained previously (Chap. II B) the full C-R model Ar/C-R has to be used to obtain both a satisfactory diagnostics of the plasma and the validation of any Ar/GI model used for its description. Comparison of the model theoretical results with the experimental spectra is based on the detailed Ar/C-R. Calculating of the individual population of each $4s$, $4p$ level allows for comparison with the corresponding experimental spectral line intensity, hence the global $4s$ and $4p$ populations coming from the kinetic model. This procedure also contributes to the validation of the used multidimensional codes. Here we present the main characteristics of the Ar I and Ar II spectra taken into consideration for diagnostics purposes.

A. Main Features of the Ar I Spectrum

The $4s$ and $4p$ Ar I levels are between the most extensively studied rare gas levels, due to their intrinsic physical properties and because they generate spectral lines frequently present in various applications, both in the visible ($4s-4p$) and in the UV region ($4s-3p$). Of the four $4s$ levels (two with $j_c=1/2$ and two with $j_c=3/2$ in jK coupling scheme) two are transitory and two metastable, the transitions of the latter to the ground level (GL) being forbidden and difficult to observe in experimental plasmas. This fact contributes to an increased population of these levels in comparison with most excited states, to the point that their population cannot be negligible in comparison with the population of the GL. The ionization cross sections of the excited states being considerably higher than the one of the GL, the metastable $4s$ levels, even less populated than the GL, may significantly contribute to the overall plasma ionization.

The ten $4p$ Ar I lines (four with $j_c=1/2$ and six with $j_c=3/2$) cannot directly decay to the $3p$ ground level, a fact that contribute to somewhat increase their population, although all of them can easily decay to the lower situated $4s$ lines giving sixteen jK allowed transitions²¹. These constitute the well known stronger Ar red lines around 800 nm (followed in intensity by the blue lines coming from the $4s-5p$ transitions) which significantly contribute to the $4s$ levels population. Seven among them lead to the two metastable $4s$ levels. Note that among the lower $4p$ levels, $2p_{10}$, $2p_9$, $2p_6$, the first and the last ones decay almost an order of magnitude easier to the metastable $1s_5$ than to the transitory $1s_4$, and the $2p_9$ decays practically only to the metastable $1s_5$. This fact confers a quasi-metastable character to these three levels.

It becomes evident that if we seek a better consideration of the important atomic processes present e.g. in thruster prototypes or in reentrance studies, we have to include in the models at least a collective representation of the four $4s$ and of the ten $4p$ levels, situated between the neutral Ar I GL and the ion Ar II GL. The mean values of the atomic processes concerning the simplified ‘four level’ atomic model (consisting of the Ar I GL, its continuum represented by the average of the two Ar II GL plus the two excited $4s$ and $4p$ global levels) have been calculated from the data corresponding to the 14 individual lines and the two levels constituting the Ar II GL. In the Fig.1 the averaged $3p^53d$ configuration is also given. It can be optionally used because it easily decays to the GL and to the $4p$ configuration. Interestingly, in the often used LS coupling description, there is a strong mixing of the transitory $4s$ levels 3P_1 ($[3/2]_1$) and 1P_1 ($[1/2]_1$) ($1s_4$ and $1s'_2$ correspondingly in the Paschen notation) and of the $4p$ 3D_1 ($[3/2]_1$, $2p_7$), 1P_1 ($[1/2]_1$, $2p'_4$) and 3P_0 ($[1/2]_0$, $2p_5$), 1S_0 ($[1/2]_0$, $2p'_1$) levels. Traditionally, levels are primed whenever belong to the $1/2$ parent core.

B. Main Features of the Ar II Spectrum

The features of the Ar II structure are analogous to the one of Ar I, being somehow more complex⁶. In fact, although the aforementioned Ar II GL is composed from two levels, its continuum (Ar III GL) is composed from five levels, thus ordering the levels of the Ar II spectrum according to five different parent cores (³P₀, ³P₁, ³P₂, ¹S₀, ¹D₂). The importance of the multiplets in the Ar II spectrum is analogous to this of the Ar I, but with the 4p configuration situated higher than the 3d one, as shown in the Fig. 1. Consequently, the 3d configuration is split for Ar II in two parts, one transitory and one metastable, increasing by one the number of mean levels used in ArI,II/C-R. Also, although the Ar III levels belong naturally to five cores, they have been here collected to only two blocs.

C. Optical Diagnostics Based on Comparison of the Experimental Results with the Theoretical Spectra

Results of our Ar/C-R theoretical model were validated using experimental spectra obtained in the University of Ioannina with an hollow cathode lamp⁶. The mean values corresponding to the 4s, 4p (and 3d) configurations of the Ar I and Ar II spectra can be directly compared with the theoretical line intensities from Ar/C-R model. Line intensities in the experimental spectra obtained from the hollow cathode plasma are comparable to those given by our Ar/C-R theoretical model for a T_e in the 1 eV to 2 eV region.

V. Conclusion

The proposed ArI,II/C-R model constitutes a significant simplification of our previous Ar plasma C-R model Ar/C-R used for the optical diagnostics of the SPT-50 prototype, both in the number of the considered ionization stages and in the number of the contained excited states of each ionization stage, which are here all averaged and pertain only to lowly excited species. Used in conjunction with our full Ar/C-R model and a multidimensional Ar/GI model allows for detailed diagnostics of the modeled plasma and provides an indispensable tool for validating the global plasma modeling. In so doing, the calculated total population of each averaged level of the ArI,II/C-R model was shared according to our full Ar/C-R model results, in order to infer the theoretical intensities of the observed real transitions needed for diagnostics. The proposed simplified ArI,II/C-R model is to be used for validation of the various Ar/GI models.

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